InversePELMO

A tool to perform

inverse modelling studies with PELMO 4.0

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1. Summary

A software called *InversePELMO* was developed that can be used to perform inverse modelling studies with PELMO using the results of higher tier outdoor studies (e.g. lysimeter experiments) as input. This is done in order to obtain key parameters for leaching models such as Kfoc (Freundlich sorption constant related to organic carbon) and DT50 (degradation time to 50%). Aim of such a study is on one hand to get a deeper look into the processes that led to a certain lysimeter result. On the other hand inverse modelling studies can be used to improve the standard modelling on tier 1 by considering additional information from higher tier studies. The results of *InversePELMO* can be used to make

- Predictions about the most likely behaviour if the lysimeter study had been conducted over a longer time period,
- Translations of the lysimeter results to a different situation with respect to the environmental conditions (e.g. different climate),
- Translations of the lysimeter result to a different situation with respect to the application pattern of the substance (e.g. change of the rate),
- Use of optimised parameter settings for a refined standard tier 1 simulation

Test simulations are performed in order to check the suitability of *InversePELMO* for the above mentioned aims. The example simulations with two different test data sets demonstrate that the link between *InversePELMO* and PELMO works sufficiently and leads to adequate descriptions of the processes occurred in lysimeter studies.
InversePELMO guides the user to a sequential process including first the calibration of soil hydrology followed by the optimisation of the substance fluxes. The user can stop the inverse modelling study at any times, exit *InversePELMO* and continue at a later time where he left. All inverse modelling studies are saved as projects and can be re-evaluated at a later time. The quality of the optimised parameters is reported according to the recommendations of FOCUS degradation kinetics (e.g. chi²-test, t-test).

2. Background

Within the registration of pesticides for all active compounds and metabolites concentrations in the environment (soil, groundwater and surface water) have to be calculated. This is done using different computer models such as Exposit (UBA 2011), PELMO (Klein 1995, Jene 1998, FOCUS 2009), EVA (Holdt et al. 2011), ESCAPE (Klein 2008) considering the results of different studies on degradation and sorption of these compounds in soil. Normally, laboratory studies are performed to get the input parameters for the models considering the recommendations of FOCUS (e.g. FOCUS 1997, FOCUS 2000, FOCUS 2006). Alternatively, the necessary input parameters can be also obtained based on outdoor studies (e.g. field dissipation studies).

Recently, the new FOCUS groundwater group suggested a third methodology for the input parameter setting (FOCUS 2009). The idea is to analyse outdoor studies, especially lysimeter studies, using the „inverse modelling technique which allows the estimation of sorption and degradation parameters within a single step. For this procedure an optimisation tool - in this project the program PEST (Watermark 2005) - has to be combined with a leaching model (in this project PELMO 4).

Aim of inverse modelling studies is to find the KOC and DT50 values that could describe the outdoor study best considering all data recorded during the experiments (e.g. rainfall, temperatures, percolate, and substance fluxes).

However, the whole procedure is rather complicated and detailed knowledge on leaching models is needed to successfully perform inverse modelling studies. The software presented here was developed in order to make available a user friendly tool to perform or check inverse modelling studies performed with PELMO and PEST.

3. Description of *InversePELMO*

Inverse modelling studies are performed in order to obtain key parameters for leaching models such as Kfoc (Freundlich sorption constant related to organic carbon) and DT50 (degradation time to 50%) from higher tier studies (e.g. lysimeter studies) instead directly from standard laboratory studies on sorption and degradation. Aim of such a study is on one hand to get a deeper look into the processes that led to a certain lysimeter result. On the other hand inverse modelling studies can be used to improve the standard modelling on tier 1 by considering additional information from higher tier studies.
Furher questions that can be answered based on inverse modelling studies are

- Prediction about the most likely behaviour if the lysimeter study had been conducted over a longer time period,
- Translation of the lysimeter results to a different situation with respect to the environmental conditions (e.g. different climate),
- Translation of the lysimeter result to a different situation with respect to the application pattern of the substance (e.g. change of the rate),
- Use of the optimised parameter setting for a refined standard tier 1 simulation

Generally, two steps have to be conducted when performing inverse modelling studies: First, the hydrology in soil is optimised, followed by the optimisation of pesticide fate as shown in Figure 1).

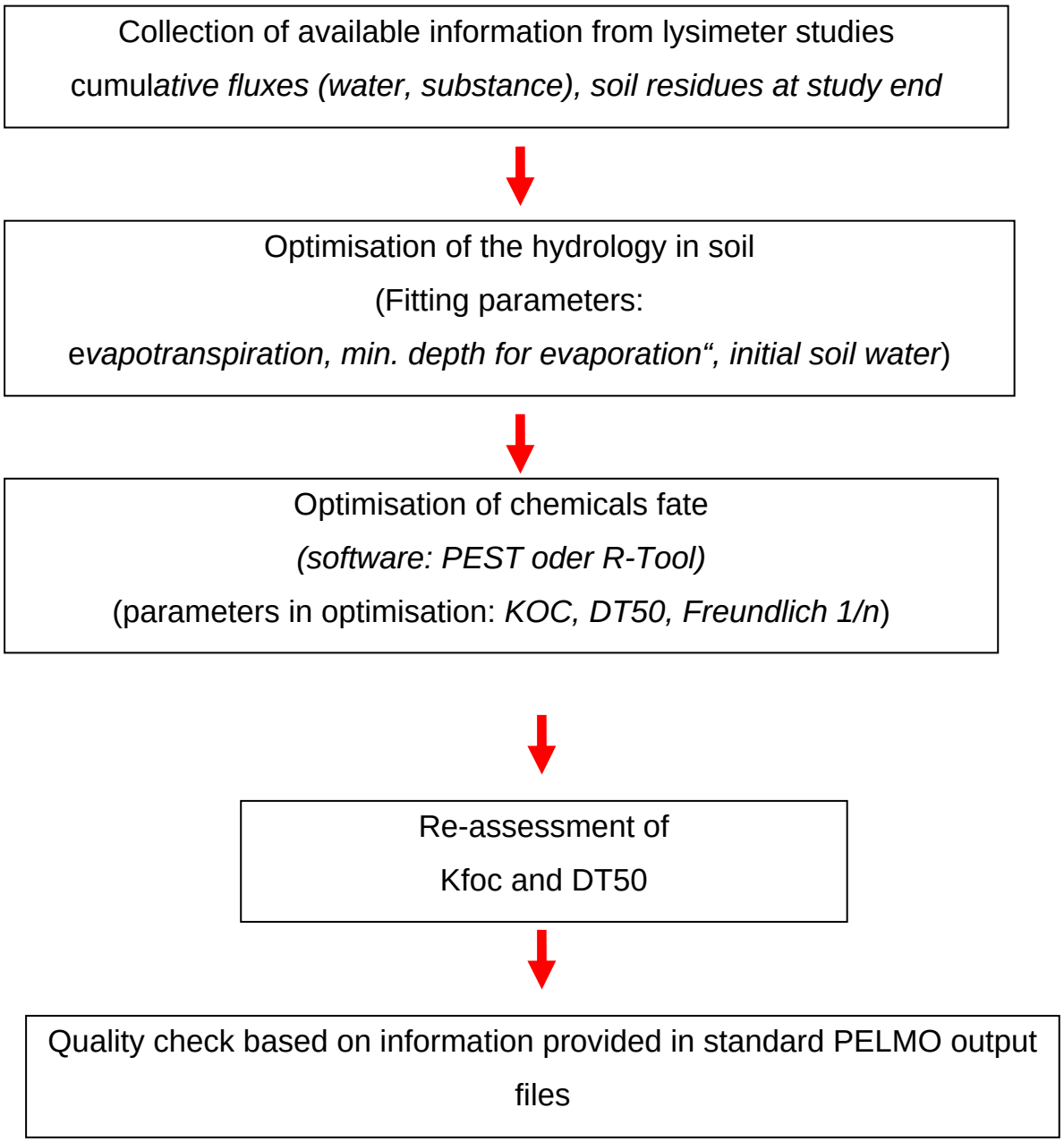
Collection of available information from lysimeter studies
cumulative fluxes (water, substance), soil residues at study end
Optimisation of the hydrology in soil
(Fitting parameters:
evapotranspiration, min. depth for evaporation“, initial soil water)
Optimisation of chemicals fate
(software: PEST oder R-Tool)
(parameters in optimisation: KOC, DT50, Freundlich 1/n)
Re-assessment of
Kfoc and DT50
Quality check based on information provided in standard PELMO output files

Figure 1: General flowchart of inverse modelling studies

As shown by the previous considerations inverse modelling studies for the calibration of lysimeter results are not totally uncomplicated but require detailed knowledge about the leaching model with its input and output file structure. Only part of this will be the creation of input data for weather and soil properties: users must be also able to manipulate pesticide input files in a dos environment. So, even if users are familiar with the normal shell and are

able to create input files for standard simulations, it will be not sufficient to go through the complex inverse modelling procedure unless special supporting software is available. Background is the additional optimisation tool in the procedure which is part of the package and which needs special input files created by the user. These additional input files are read in by this optimisation tool and used to create PELMO input files automatically by the within the optimisation sequence. Also the

Also the post processing of PELMO output files during the sequence of the inverse modelling study cannot be simply done based on the standard user shell. The optimisation software needs exact information about the location of individual simulation results (e.g. percolate at a specific day of the simulation) in order to compare predictions with experimental data.

The new shell *InversePELMO* is able to provide both programs (the optimisation tool and the simulation model) with the necessary input files in the correct format. *InversePELMO* has also a built-in module to perform standard statistical tests to check the quality of the optimisation such as the determination of the FOCUS error at which the chi² error passes described in FOCUS (2006).

The optimisation tool selected for *InversePELMO* was PEST version 7.2 (Watermark 2003) because it met all criteria necessary to combine it with PELMO in a DOS environment. It was also tested that PEST works under all relevant windows systems (Windows XP, Windows VISTA and Windows 7, 32 bit as well as 64 bit version).

4. Working with *InversePELMO*

4.1. Installing *InversePELMO*

To install *InversePELMO* following steps have to be done:

1 Install PELMO 4 (if it has not been done so far)
2 Call *InversePELMO*_setup.zip
3 Select a directory and start unzipping the files into a temp-folder
4 After unzipping close *InversePELMO*_setup.zip
5 call setup.exe in the folder where the files were unzipped

InversePELMO may be un-installed using first the standard MS-Windows un-install tools provided in the “Control Panel” under “Add/Remove Programs”.
After successful installation the main form of *InversePELMO* will appear when calling the file *InversePELMO*.exe (Figure 3).
If you call *InversePELMO* for the first time, please make sure that the path to PELMO which is given on top of the main form is correct. You can modify the path after clicking at the input field on the form.

4.2. File handling between *InversePELMO* and PELMO

PELMO is the standard model for doing leaching simulations for registration purposes in Germany (Holdt et al. 2011) and in Europe FOCUS (2009). However, PELMO with its normal shell is not designed to perform inverse modelling studies because these studies require several model runs including automatic modification of input files based on the comparison with experimental results.
A scheme that shows the file handling is presented in Figure 2 for an optimisation of pesticide properties based on cumulative fluxes in the leachate. All pesticide and application parameters are gathered in text files with extension “psm”. The scenario input data can be found in files with extension „sze”. Before starting the inverse modelling calculation a first simulation (with initial conditions for either the soil hydrology or pesticide properties) should be prepared using the normal shell (which can be called directly from *InversePELMO*).
The optimisation itself is done automatically by *InversePELMO*.
As shown in Figure 2 *InversePELMO* calls PEST which then reads the control file pest_pesticide.pst with all information about the parameters considered for the optimisation including their initial values and their allowed ranges. Also the experimental data (e.g. cumulative fluxes) can be found in pest_pesticide.pst.

According to the information in pesticide.tpl *PEST.exe* is able to create pesticide input files (pesticide.psm) for PELMO including the correct position for the input parameters used in the optimisation. After this file has been written PEST calls PELMO for a simulation. To make the interface between PELMO and PEST more stable a second program is always executed after PELMO (in the example presented in Figure 2: PELMO_results_pesticide.exe) which gathers the important simulation results (e.g. calculated cumulative pesticide fluxes) and writes them into the file pest.plm. After both programs (PELMO and PELMO_results_pesticide.exe) are finished PEST gets control again and will read the important simulation results listed in pest.plm (instructions for PEST to read pest.plm is given in pest.ins). According to the simulation results a new iteration is initiated with new DT50 and Kfoc data for the optimisation until the optimisation is finalised.

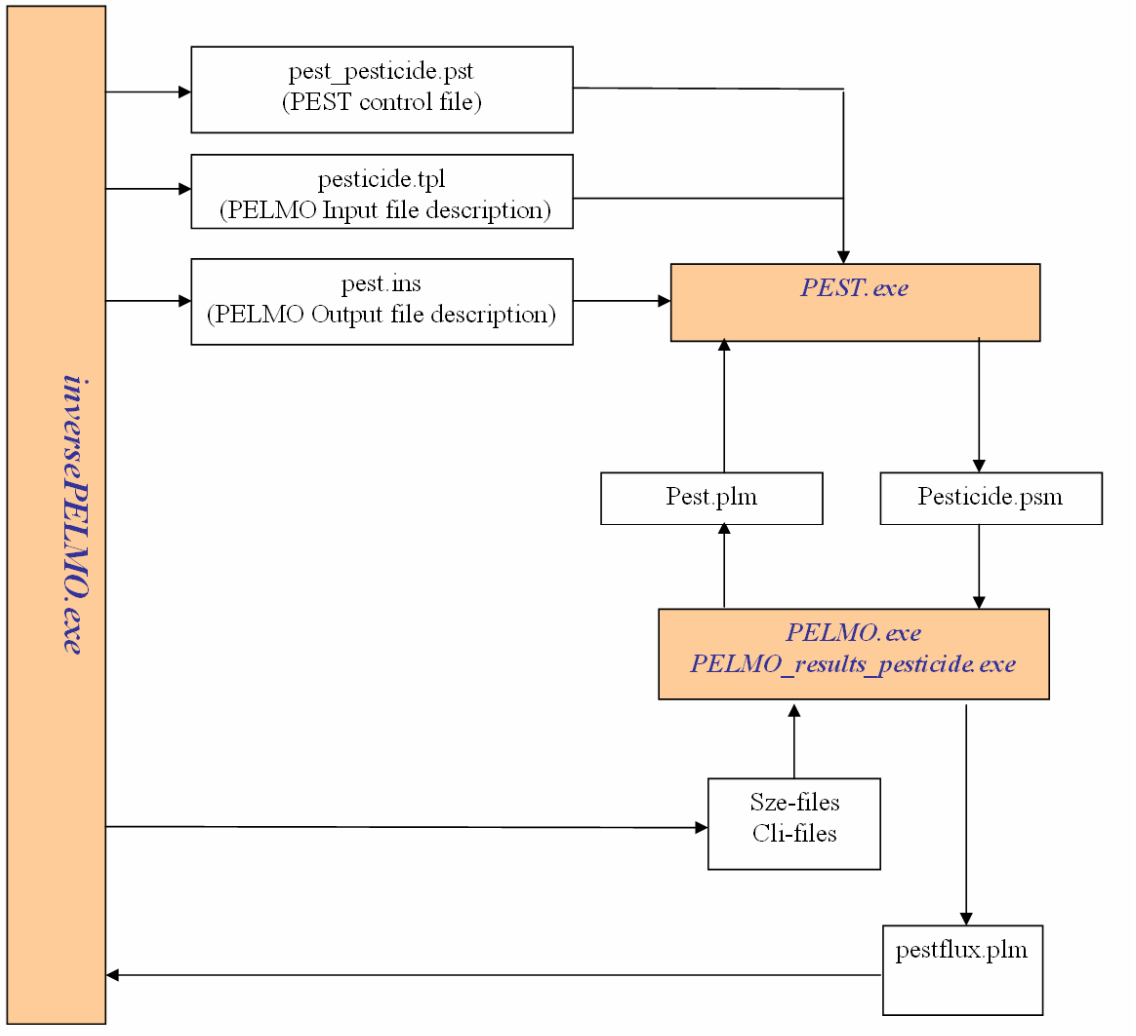

Figure 2: Flow chart: File handling of a flux optimisation with *InversePELMO*

4.3. *InversePELMO*: Main form

After successful installation the main form of *inversePELMO* appears as shown in Figure 3.

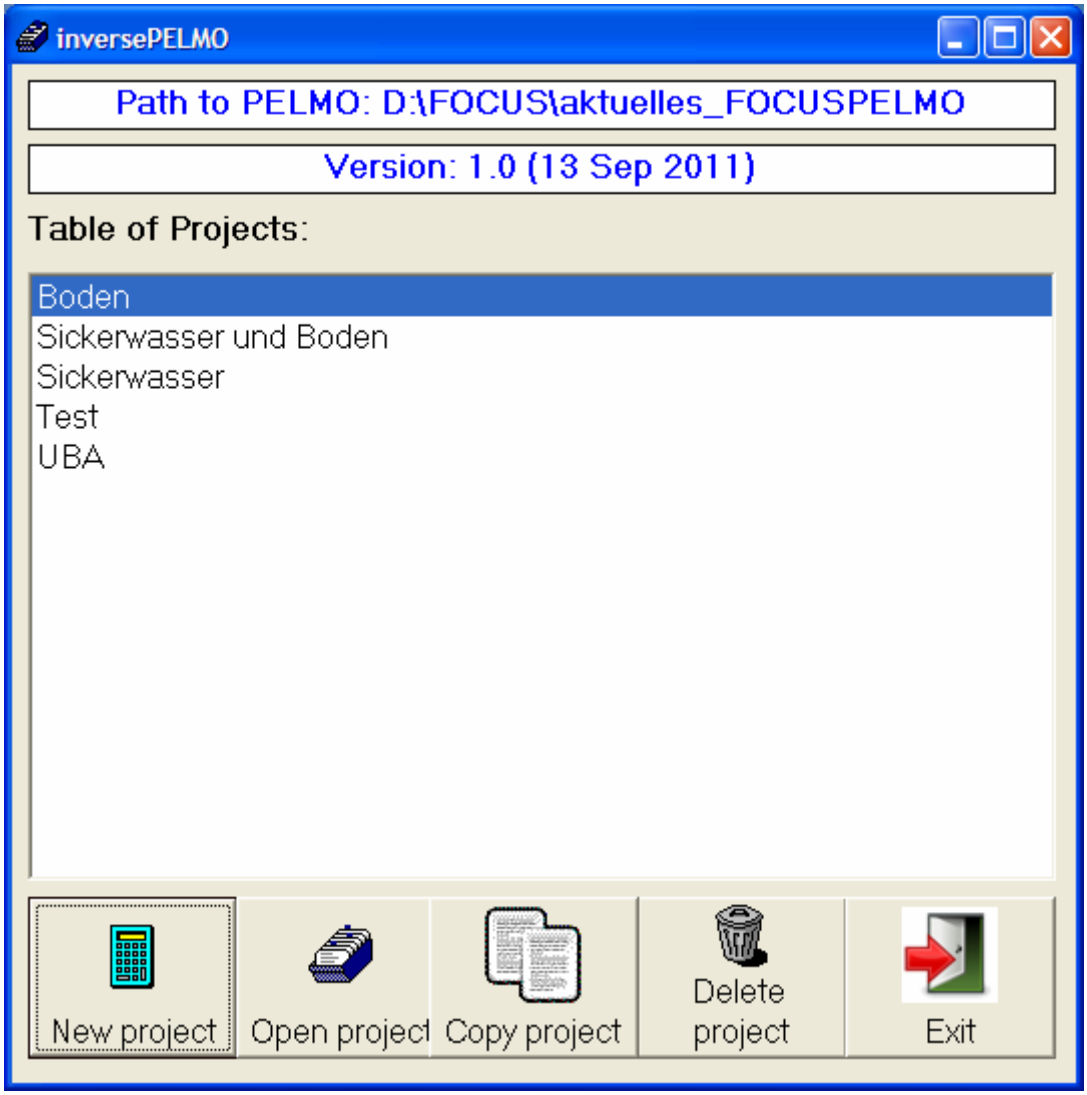

Figure 3: *InversePELMO*: Main form

4.3.1. Status Information

Two fields on top of the form give information about the path to the FOCUS PELMO installation and about the current version of the software. If the user clicks at the path a form will be loaded to change the current setting as shown in Figure 4.

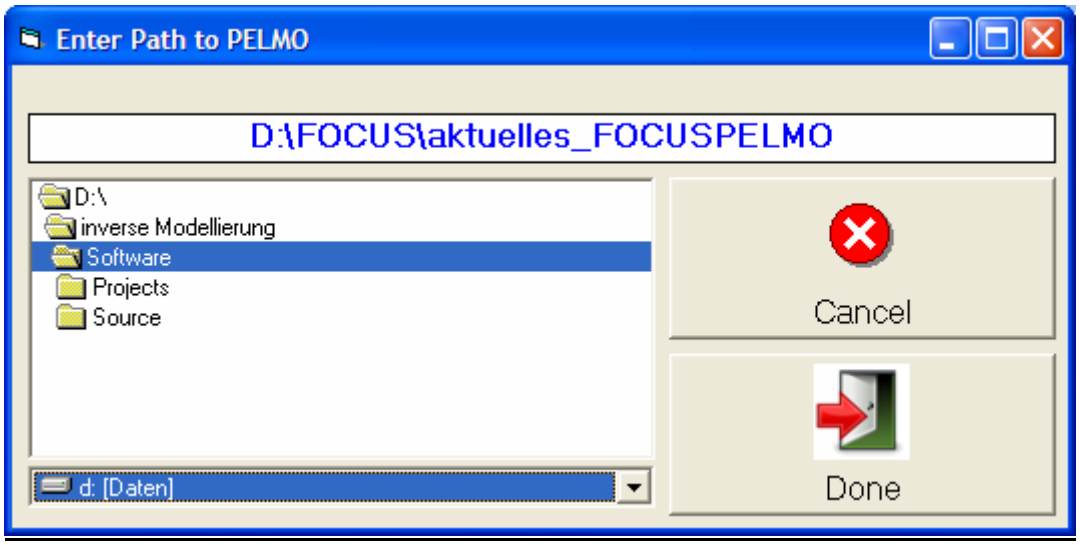

Figure 4: *InversePELMO*: Path to FOCUS PELMO

After a mouse click at the information field on current the software version the form shown in Figure 5 will appear.

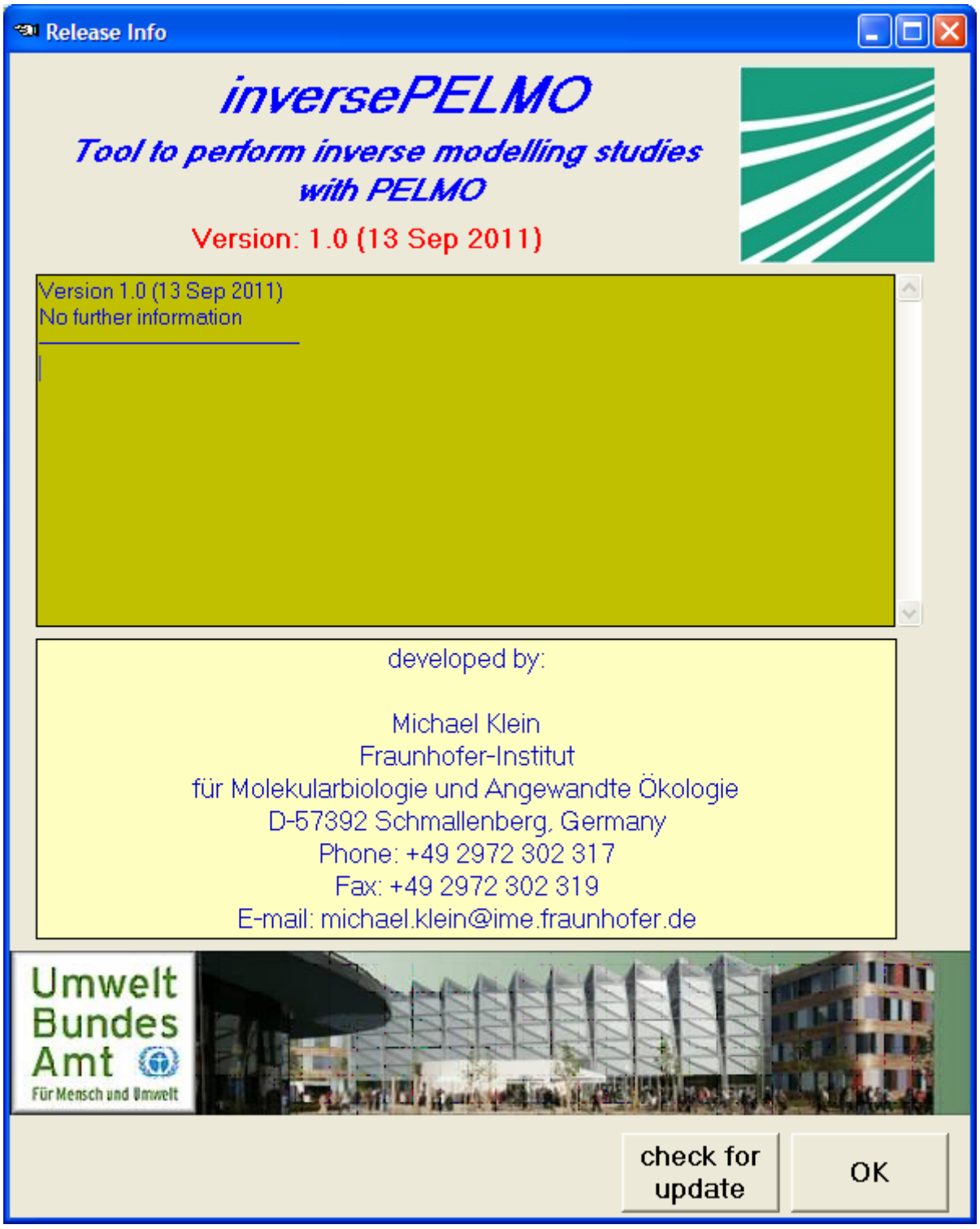

Figure 5: *InversePELMO*: Release information

On this form the button “check for update” can be used to look for new releases of *InversePELMO*.

4.3.2. Project list

On the left side the form shows a list of all inverse modelling studies (= projects) available. Information for each project is gathered in a respective directory of the same name. All project directories are located in the folder “projects”. Usually, a project folder has following content:

- Up to 5 executables: the optimisation tool PEST (pest.exe), the simulation model PELMO (pelmo400.exe) and its post processors “pelmo_results_water.exe” (gathering information on simulated percolate), “pelmo_results_pesticide.exe” (gathering information on cumulative substance fluxes) and “pelmo_results_soil_profile.exe” (PELMO gathering information on soil concentrations).
- Standard PELMO input files: the normal pesticide and scenario input files with extension “.psm” and “.sze”, respectively. Furthermore, at least one climate data file (extension “.cli”) and the normal control file of PELMO called “pelmo.inp”
- Standard PEST control files: “pest_pesticde.pst” and “pest_water.pst”, scenario.tpl (information how to create PELMO scenario input files), pesticide.tpl (information how to create PELMO pesticide input files), pest.ins (information how to extract simulation results out of PELMO)
- Standard PELMO output files: echo.plm, wasser.plm, chem.plm, plot.plm
- Specific PELMO output file containing information used by PEST: perkolat.plm, flux.plm, soil concentrationXX.plm (XX= number of soil layer e.g. soil concentration01.plm)
- MS-DOS batch files “Run_water.bat” and “Run_pesticide.bat” created by PEST, used to start the PELMO simulation and to prepare the simulation results for PEST
- PEST output files: e.g. “pest_soil_concentrations.rec” with detailed information on the optimisation. Additional files with the same name, but different file extensions are created by PEST such as “pest_soil_concentrations.jac” with other information (e.g. about parameter sensitivity)

The files in the project folder should be not removed manually by the user because it may lead *InversePELMO* to crash when scrolling through the project list.
After a double click at one of the items in the list box (or when using the button “Open project”) *InversePELMO* will load the project.

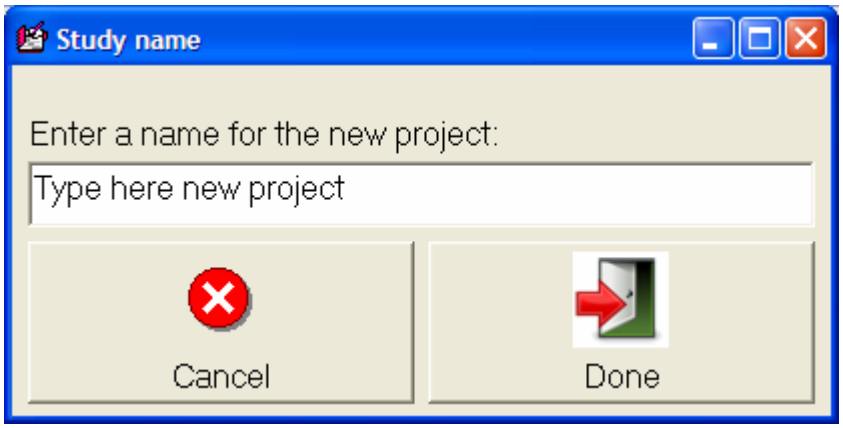

Figure 6: *InversePELMO*: New project

4.3.3. Command buttons

Five buttons are placed on the main form allowing direct access to important functions of *InversePELMO*:

New project: This button calls the dialogue shown in Figure 6 to name the new project. It is not possible to use the name of an existing project. If existing projects should be overwritten, please delete the old project first. After a click at “Done” the optimisation form will appear (see section 4.4).

- Open project: After a click at this button *InversePELMO* will load all details of the project. The user may have a look at the current parameter setting, improve the optimisation or produce tabular or graphical output (see also the section on new project). More information about project can be found in section 4.4.
- Copy project: A click at that button will first open a form where the name for the new project can be entered (see Figure 6). Then, all information of the selected project is copied into a second folder. The option can be useful when a certain modification of an existing inverse modelling study should be performed without loosing information of the current status and without going through whole sequence of an inverse modelling study.
- Delete project: After a click at this button the selected project will be removed from the system. To avoid accidental deleting the user has to confirm the command in an additional message box.
- Exit: A click at that button will terminate *InversePELMO*.

4.4. *InversePELMO*: Optimisation

This form is used for new projects (see Figure 7) as well as existing projects (see Figure 8). However, if a new inverse modelling study should be performed a certain sequence has to be followed. A red arrow is used to guide the user through this process. For the same reason most of the buttons are disabled at the beginning.

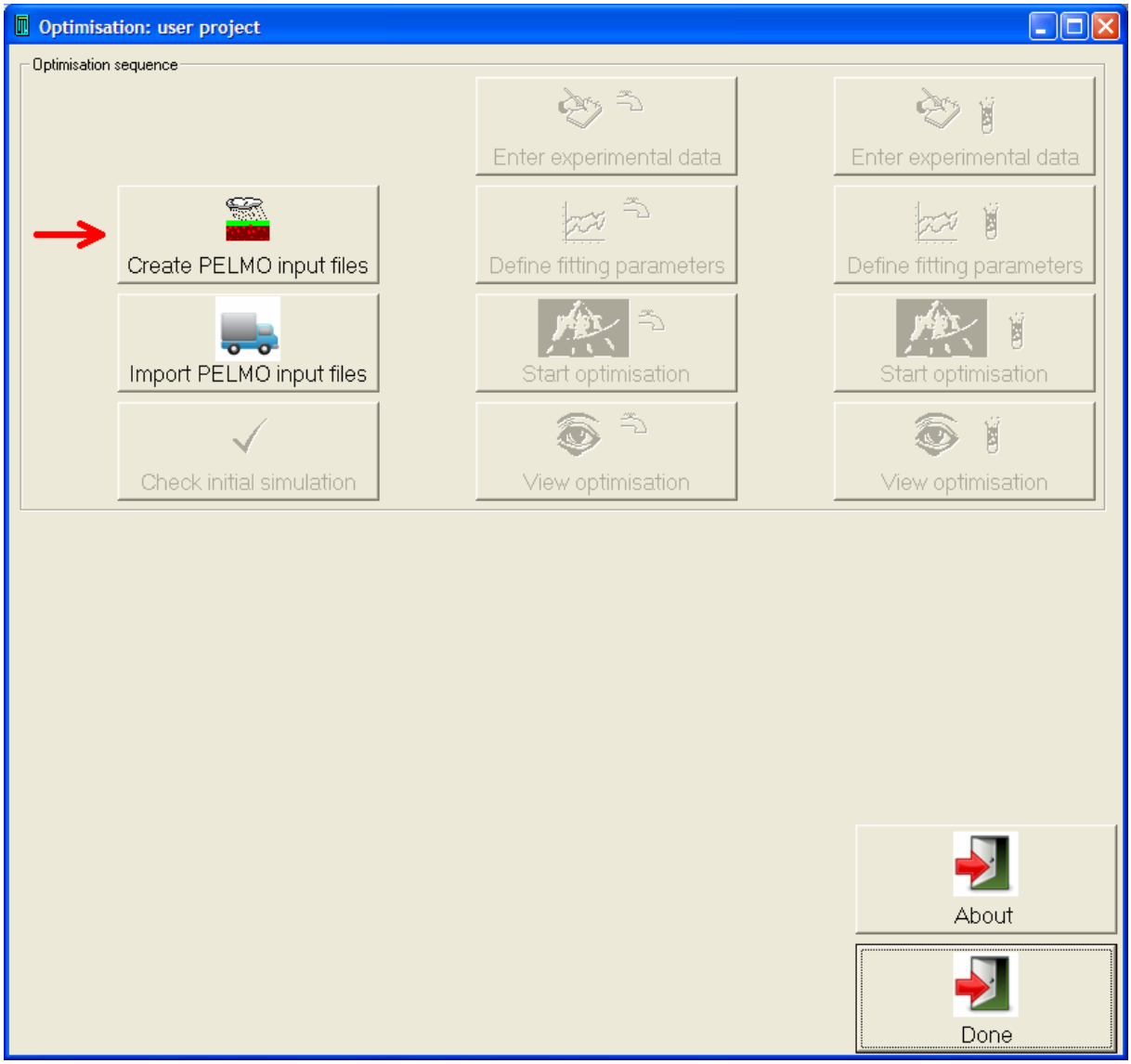

Figure 7: *InversePELMO*: Optimisation form (new project)

However, these limitations do not held for inverse modelling studies previously performed (see Figure 8).

If the user did not go through all steps of the study so far last time, some buttons may be still disabled when the project is called again. The red arrow will then indicate where to continue.

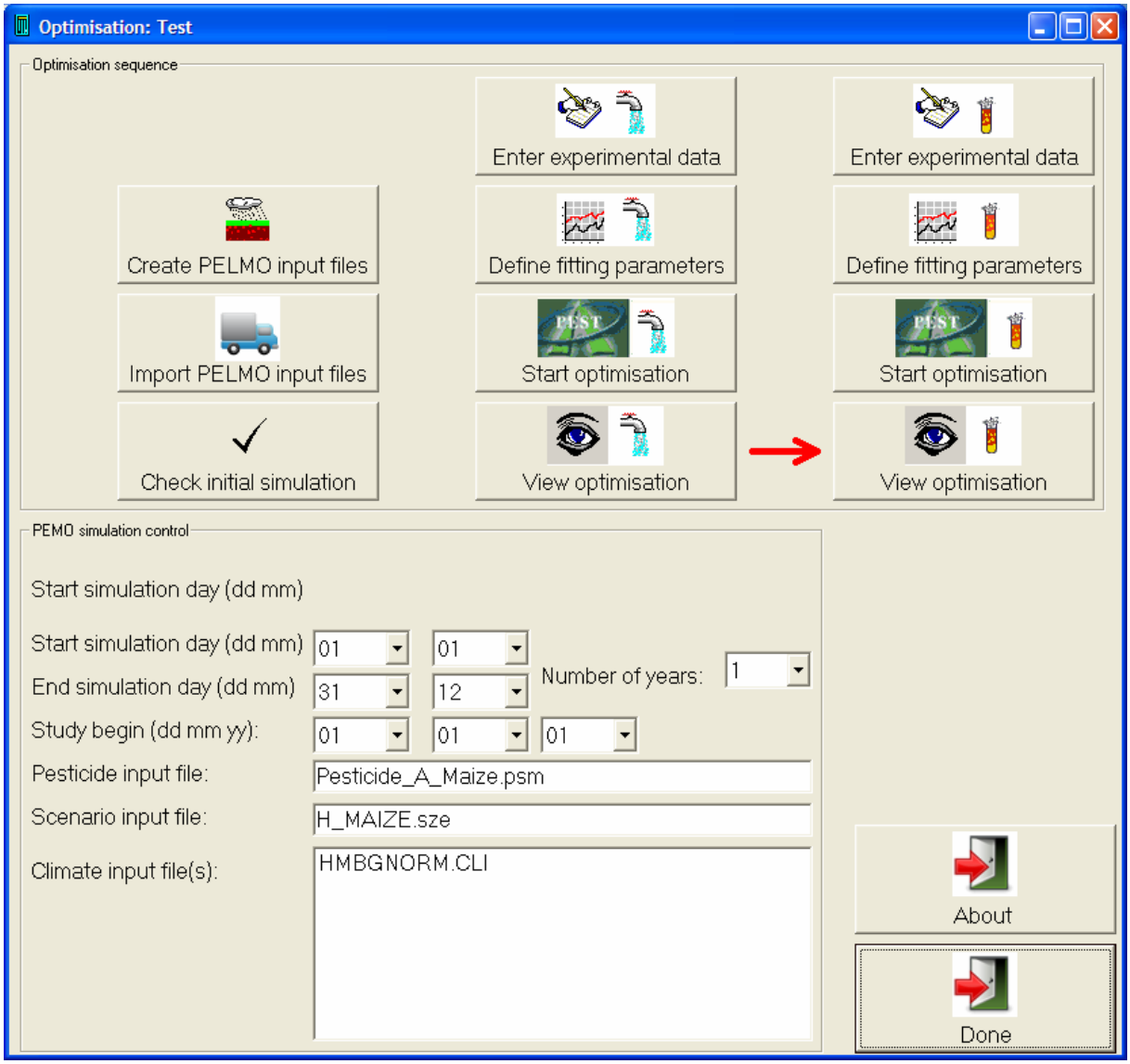

Figure 8: *InversePELMO*: Optimisation form (existing project)

In the following detailed information about the sequence of doing inverse modelling studies with *InversePELMO* is given, assuming that a new project has been created.

4.4.1. Step 1: Create PELMO input files

In the first step the necessary input files for the inverse modelling study has to be created. The click at the respective button (see Figure 7) will open the normal FOUCS PELMO shell for the editing. If all scenario, climate and pesticide input files are available and FOCUS PELMO closed the red arrow will jump to the next button.

4.4.2. Step 2: Import PELMO input files

In step 2 all PELMO input files will be copied into the project folder and some additional information about the duration of the lysimeter study has to be provided. This information has

to be entered in the frame “PELMO simulation control”. The start and end date of the simulation is related to the PELMO simulation whereas the study begin is related to the start of the lysimeter study which may be different when a warming up period is considered for PELMO in order to optimise the soil hydrology.

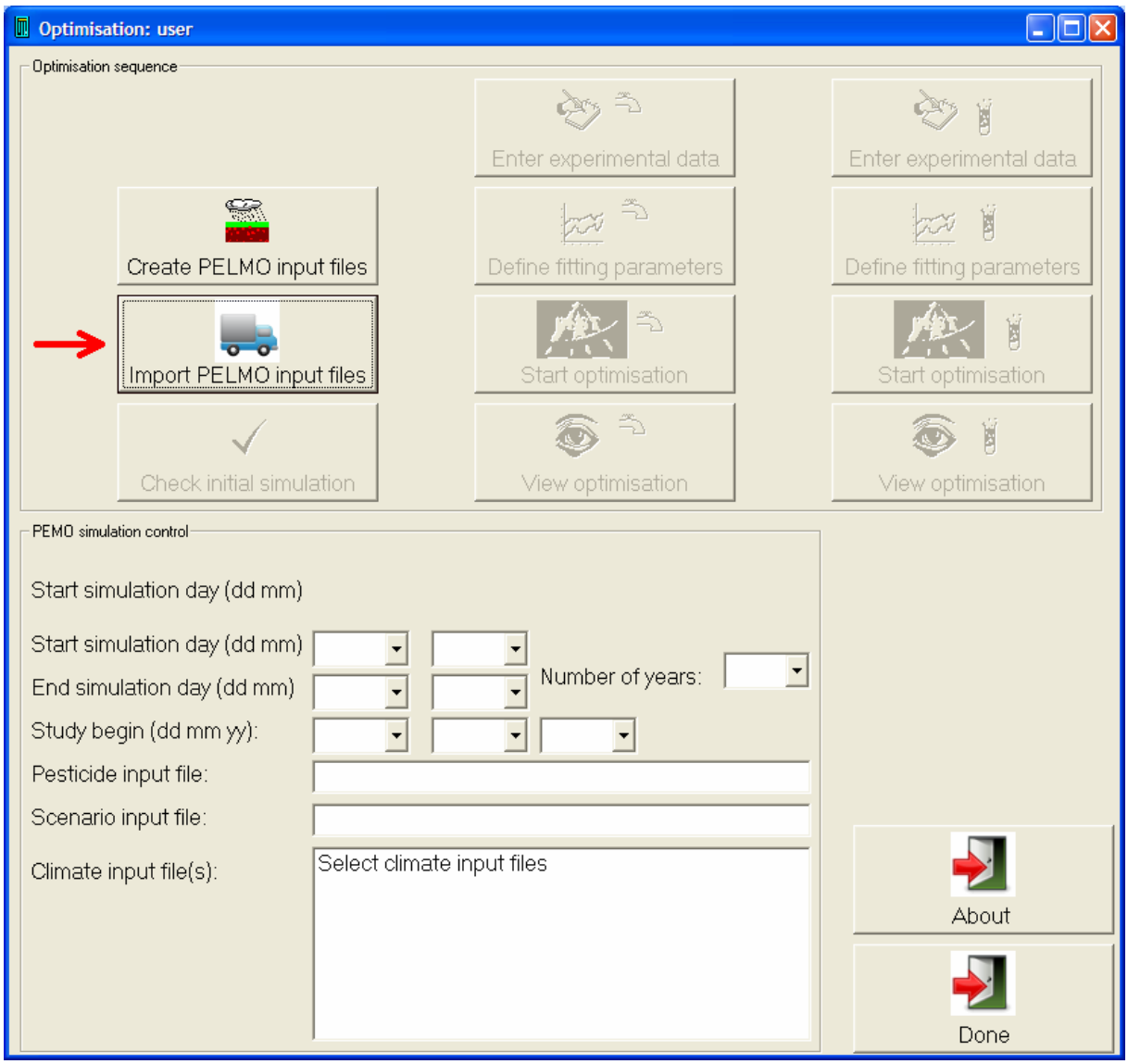

Figure 9: *InversePELMO*: Import PELMO input files

During this step also all necessary executables are copied into the project folder. That should make the documentation of the various programmes used for the analysis more transparent.

4.4.3. Step 3: Check initial simulation

After clicking at the button it is checked whether the initial simulation runs without problems. After PELMO terminates the user has to confirm that the simulation didn't quit with an error condition. Only after confirmation the arrow will move to the next button (see Figure 10).

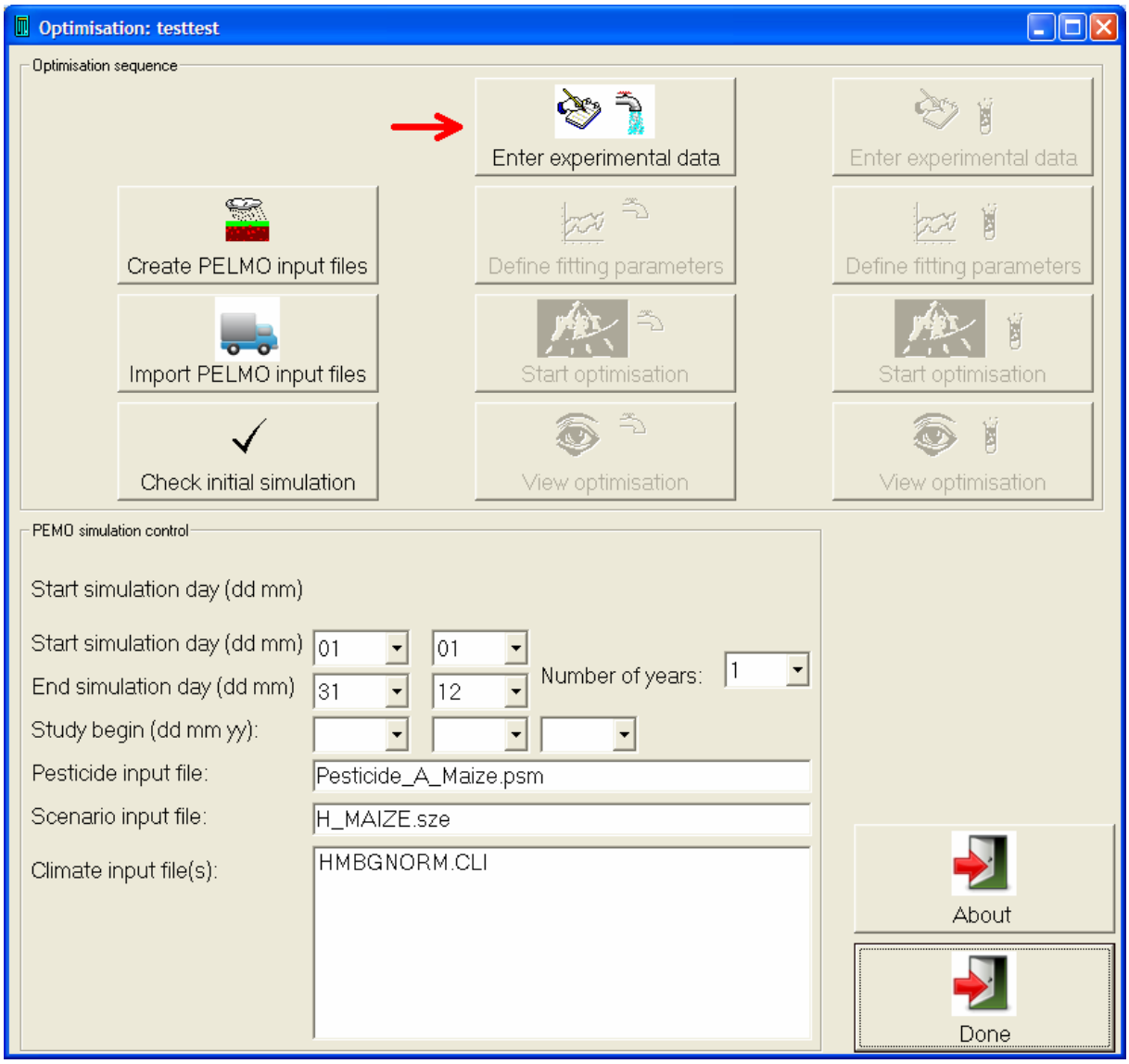

Figure 10: *InversePELMO*: experimental data (percolate)

4.4.4. Step 4: Enter experimental data (percolate)

In step 4 the experimental percolate has to be entered in a specific form (see Figure 11).

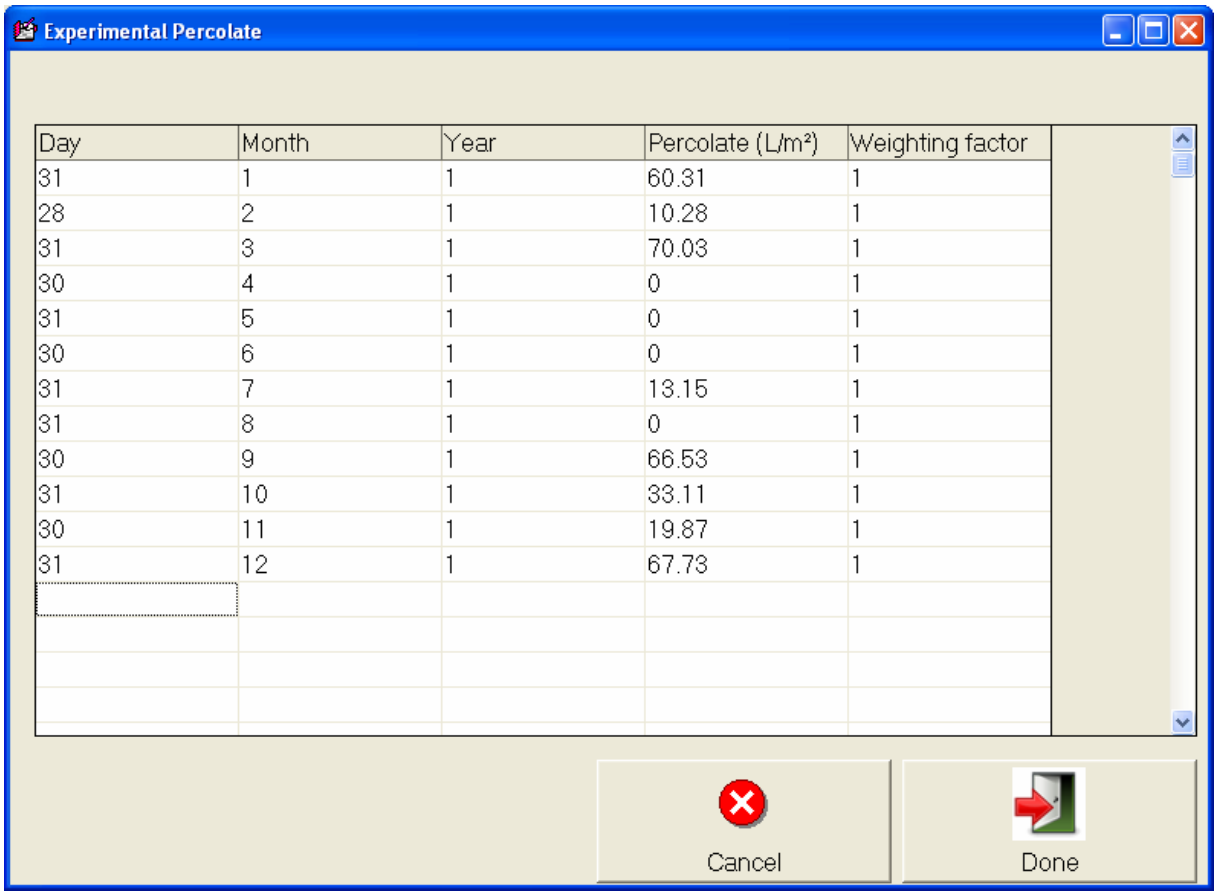

Figure 11: *InversePELMO*: Experimental Percolate

For each sampling during the study the date and the amount of percolate in L/m² is needed. The user should not enter any cumulative numbers here, because they will be automatically calculated by *InversePELMO.* If appropriate the individual sampling can be characterised by weighting factors in the final column. If the form has been filled correctly (e.g. no negative figures) it can be closed using the “Done” button and the arrow on the optimisation form will jump to the next button to enter all information about the input parameters used in the optimisation (see Figure 12). It is not necessary to type all information the user can also paste them in as a table (e.g. from MS Excel or MS Word).

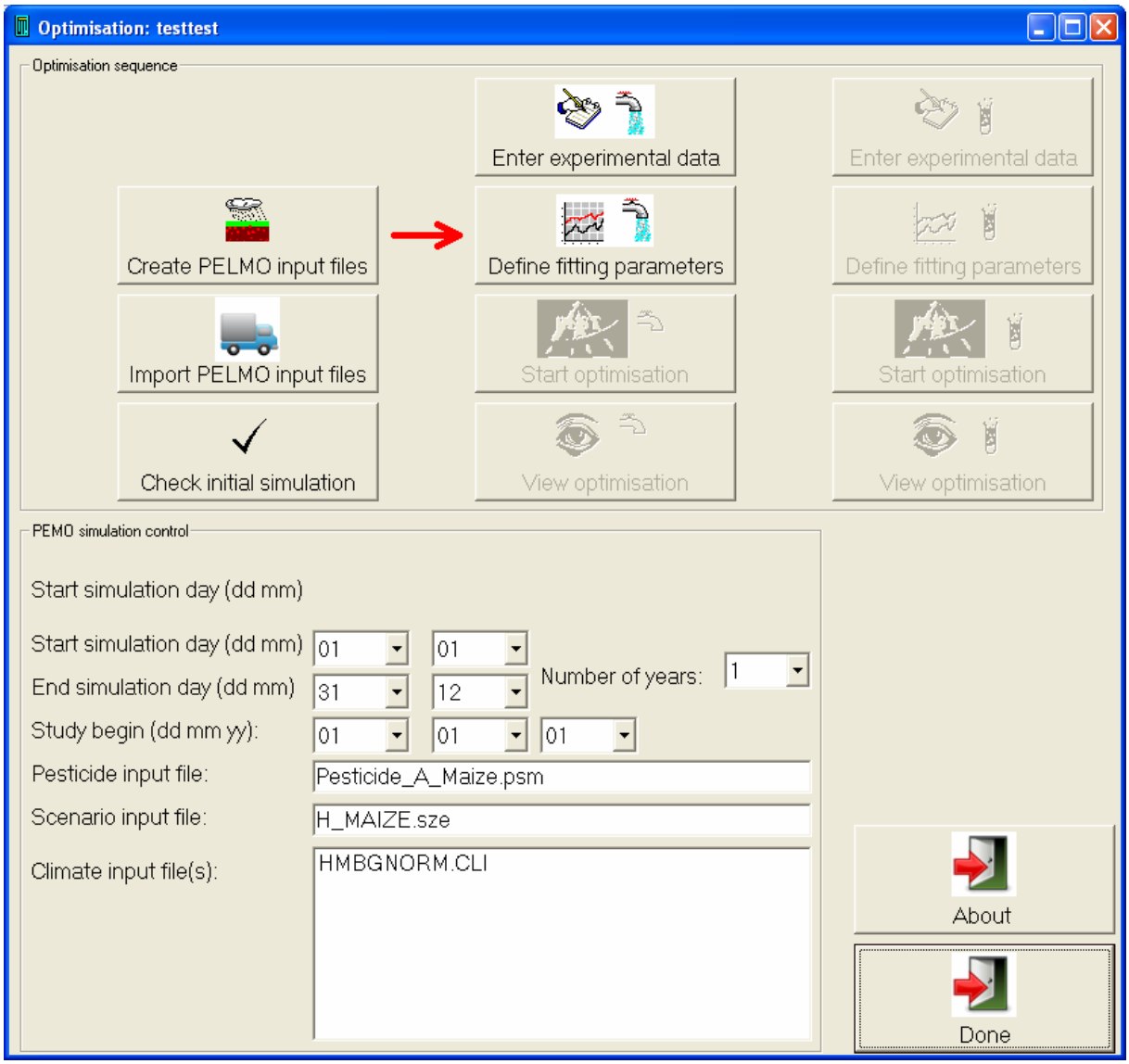

Figure 12: *InversePELMO*: define fitting parameters for the hydrology in soil

4.4.5. Step 5: Enter fitting parameter (percolate)

In step 5 the parameters used in the optimisation have to be characterised in a specific form (see Figure 13).

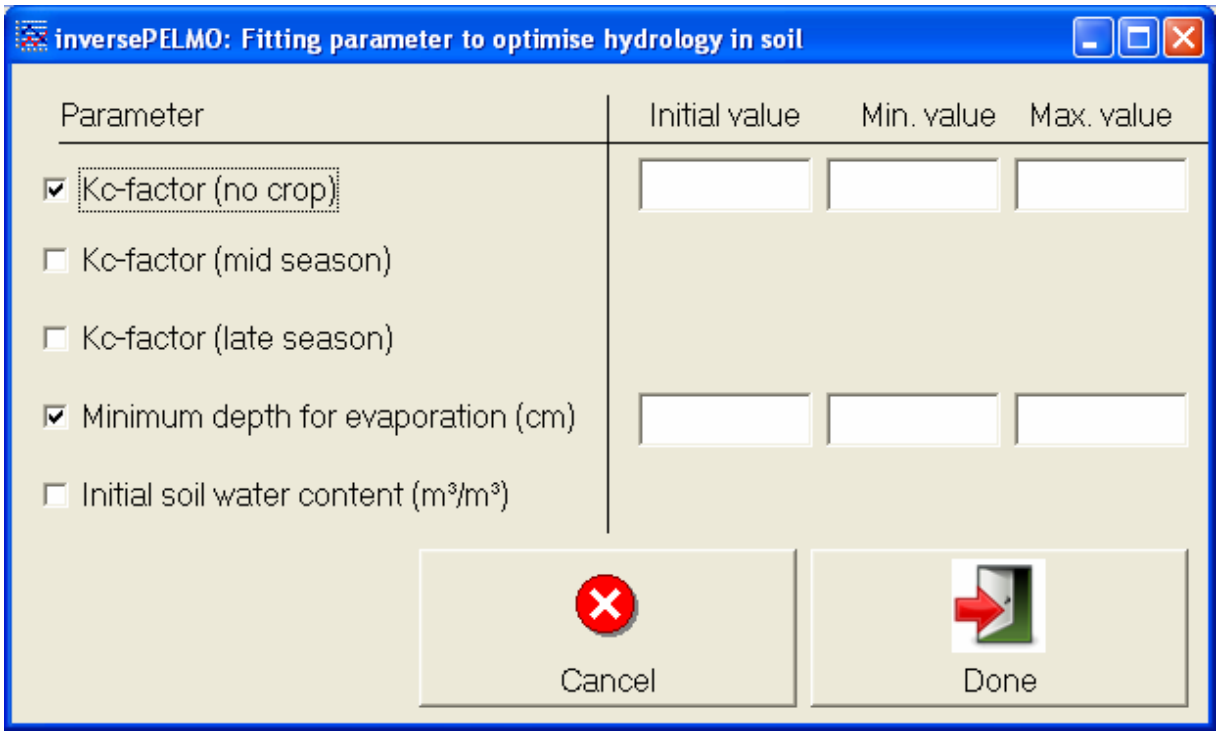

Figure 13: *InversePELMO*: Parameter for fitting the percolate

In total five PELMO input parameters influencing the hydrology in soil can be used to do the fitting.

- Kc-factor (no crop): linear correction factor for daily potential evapotranpiration when there is no crop in the field
- Kc-factor (mid season): linear correction factor for daily potential evapotranpiration when the crop is growing
- Kc-factor (late season): linear correction factor for daily potential evapotranpiration when the crop is at senescence
- Minimum depth for evaporation (cm): minimum depth for evaporation which is used independent whether or not a crop is present
- initial soil water content: soil water content at the beginning of the simulation

If parameters shall be considered for the optimisation their initial values and their range have to be specified. If a parameter is not checked the respective input fields is invisible.
If the form has been filled correctly (e.g. no negative figures, no minimum values higher than maximum values) it can be closed using the “Done” button and the arrow on the optimisation form will jump to the next button which is the button for starting the optimisation (see Figure 13).

4.4.6. Step 6: Optimisation of the hydrology in soil (percolate)

In step 6 of the sequence the optimisation is performed. During the optimisation PEST will call PELMO several times. After PEST terminated the user has to confirm that the optimisation didn't quit with an obvious error conditions.

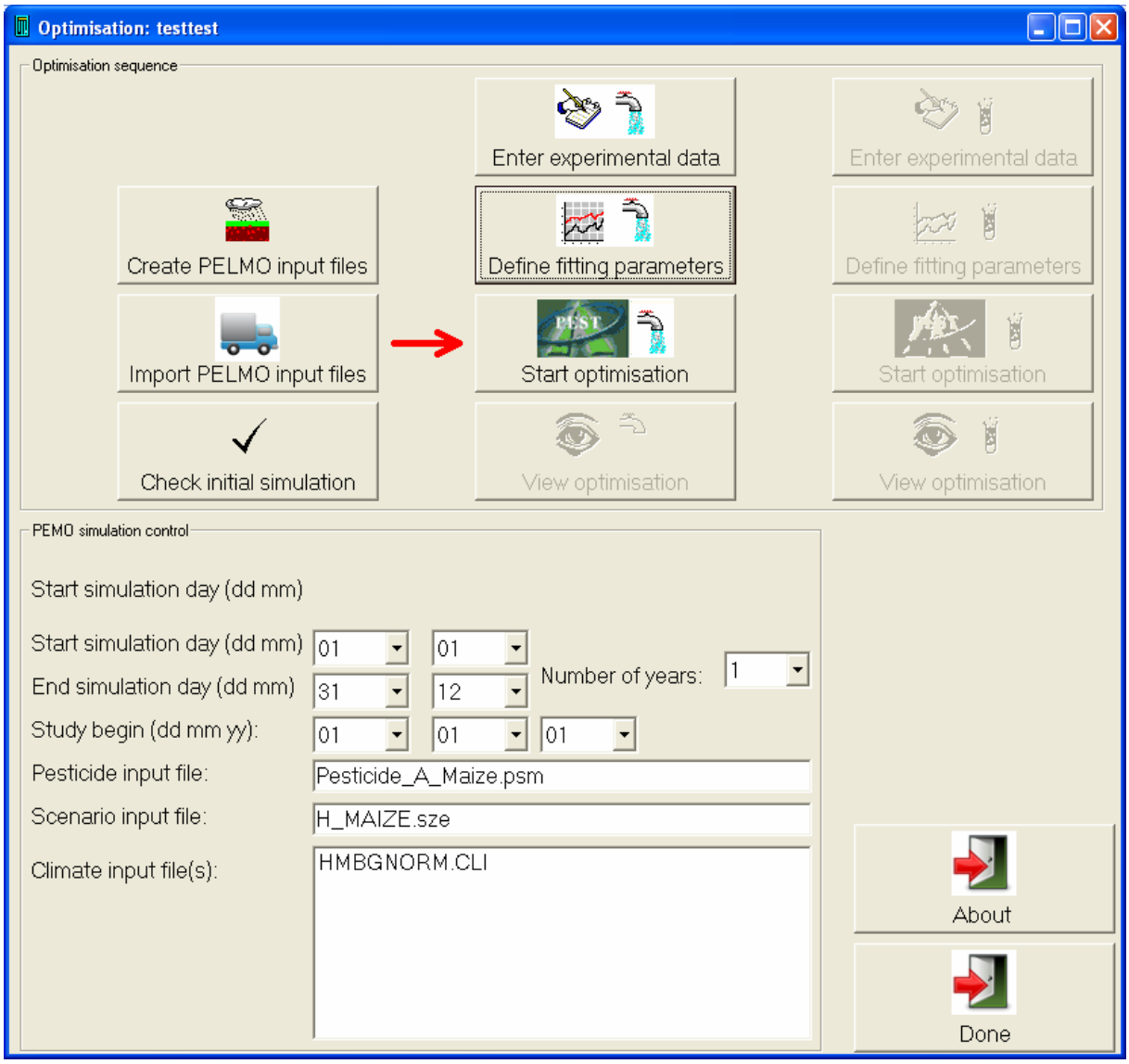

Figure 14: *InversePELMO*: start optimisation for the hydrology in soil

Only after confirmation the arrow will move to the next button (see Figure 15).

4.4.7. Step 7: View the optimisation (percolate)

In step 7 the user can evaluate the results of the percolate optimisation.

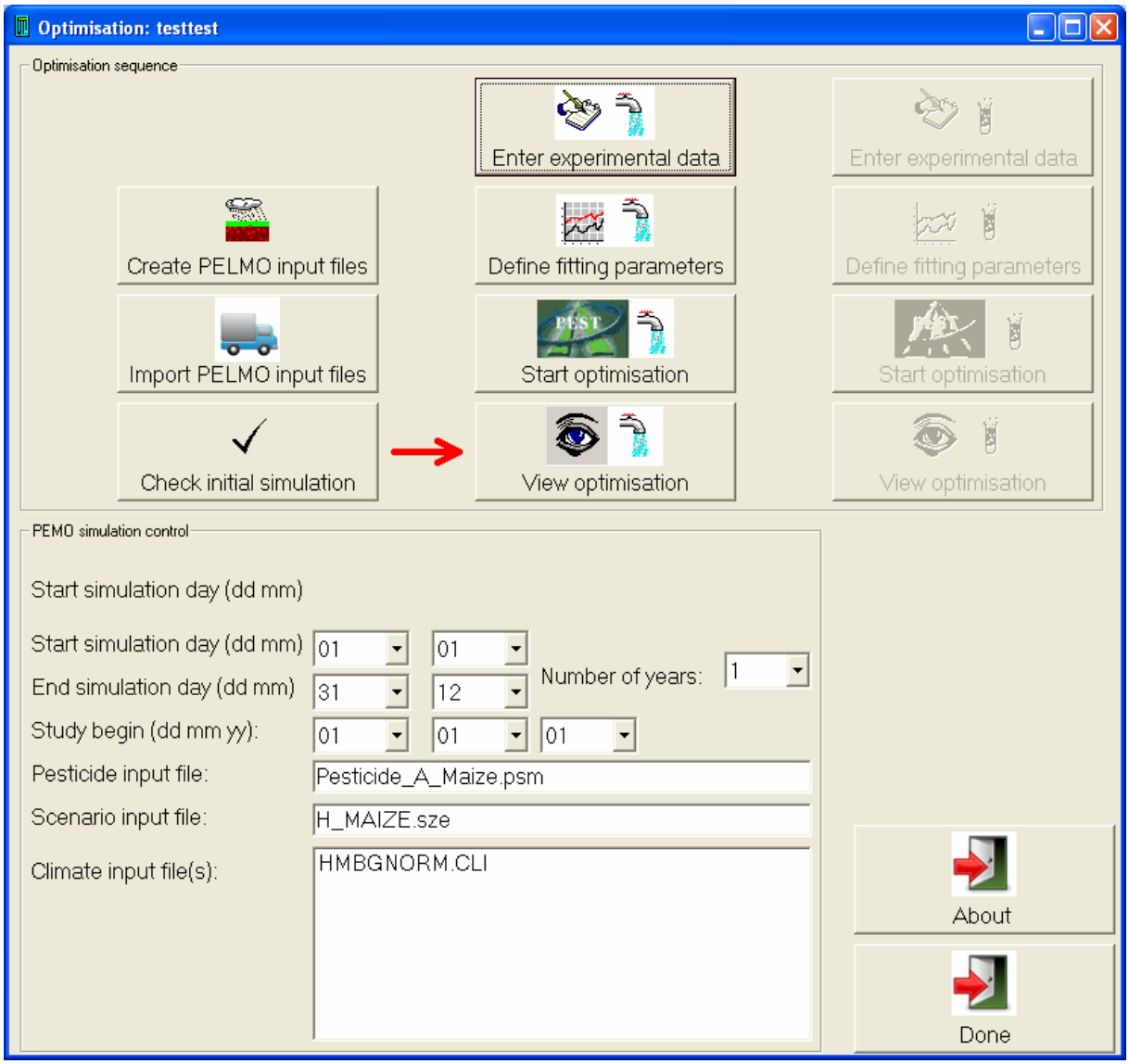

Figure 15: *InversePELMO*: Analyse the results of the optimisation for soil hydrology (percolate)

After clicking at the respective button (arrow on Figure 15) a form is loaded showing the experimental and optimised cumulative percolate graphically (see Figure 16).

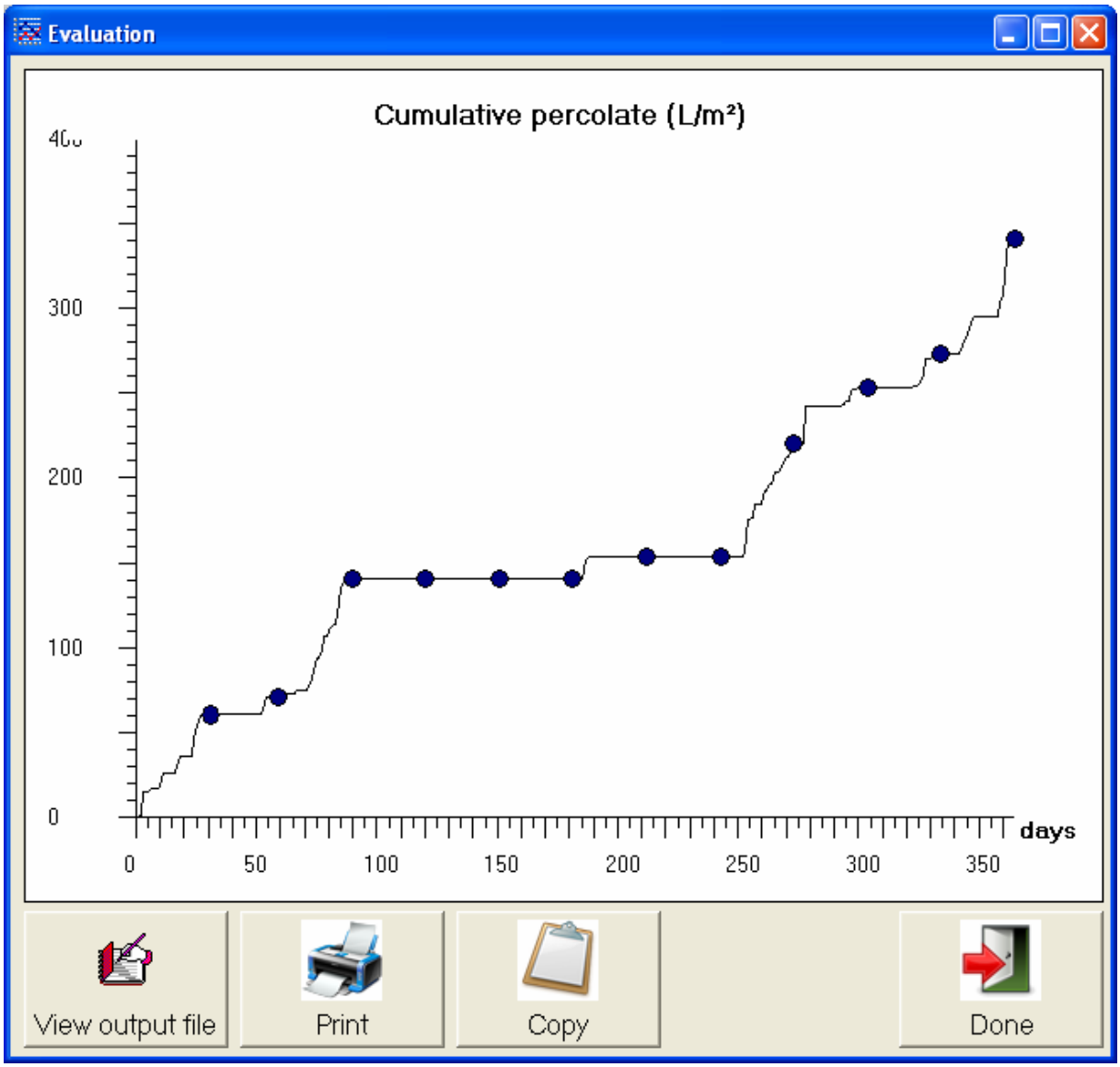

Figure 16: *InversePELMO*: View the results of the optimisation (percolate)

The circles represent the experimental data; the curve stands for the PELMO optimisation. Detailed output describing the optimisation procedure is available via the button “View output file” (Figure 17).

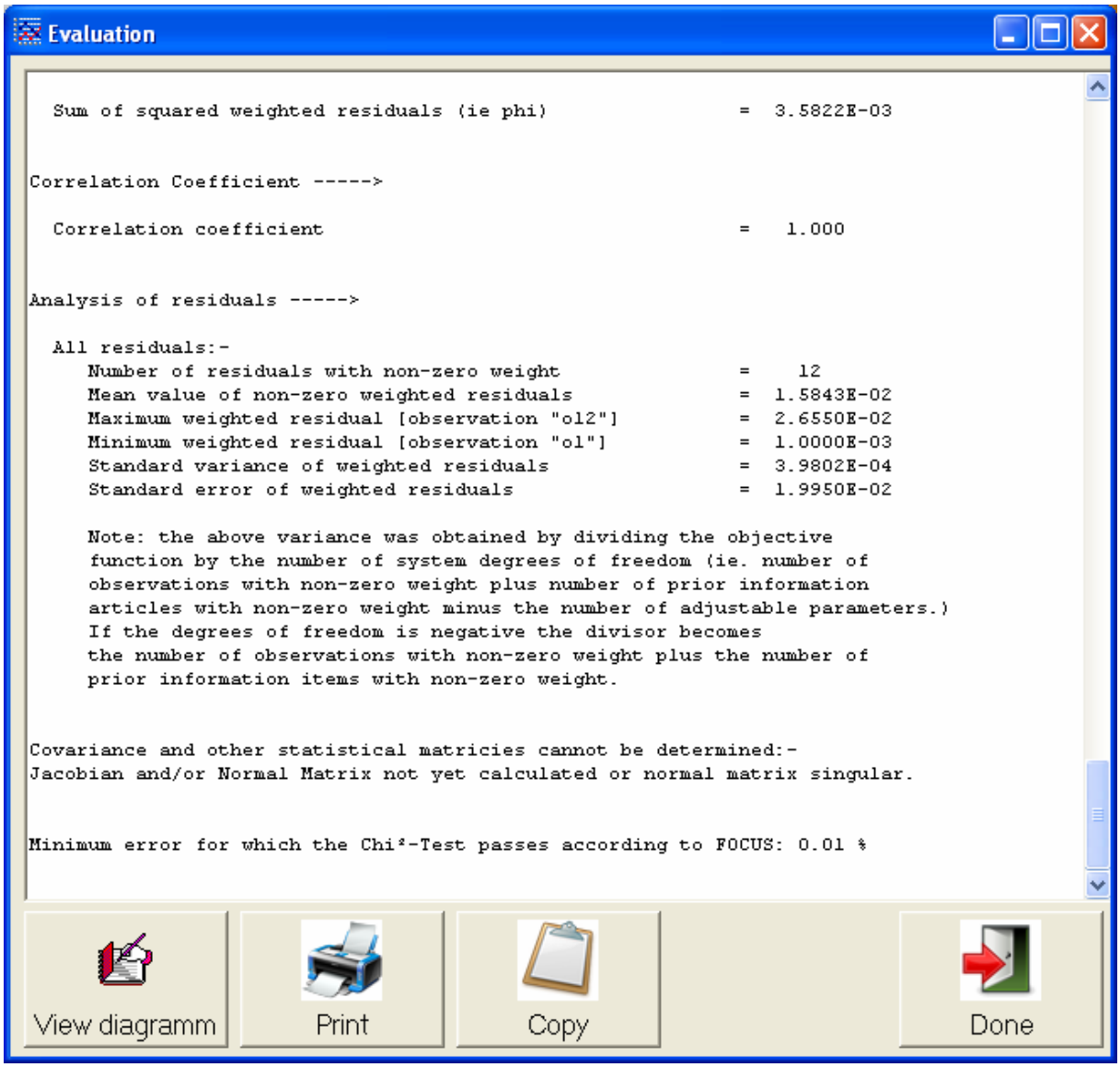
Evaluation
Sum of squared weighted residuals (ie phi) = 3.5822E-03
Correlation Coefficient ----->
Correlation coefficient = 1.000
Analysis of residuals ----->
All residuals:-
Number of residuals with non-zero weight = 12
Mean value of non-zero weighted residuals = 1.5843E-02
Maximum weighted residual [observation "ol2"] = 2.6550E-02
Minimum weighted residual [observation "ol"] = 1.0000E-03
Standard variance of weighted residuals = 3.9802E-04
Standard error of weighted residuals = 1.9950E-02
Note: the above variance was obtained by dividing the objective function by the number of system degrees of freedom (ie. number of observations with non-zero weight plus number of prior information articles with non-zero weight minus the number of adjustable parameters.) If the degrees of freedom is negative the divisor becomes the number of observations with non-zero weight plus the number of prior information items with non-zero weight.
Covariance and other statistical matricies cannot be determined:-
Jacobian and/or Normal Matrix not yet calculated or normal matrix singular.
Minimum error for which the Chi²-Test passes according to FOCUS: 0.01 %
View diagramm
Print
Copy
Done

Figure 17: *InversePELMO*: Evaluate the results of the optimisation (percolate)

The standard output file of PEST (extension “rec”) is used here, but with additional information included about the error at which the chi² test passes. The methodology is according to FOCUS degradation kinetics (FOCUS 2006). The copy button puts either graphic or the text into the clipboard, whereas the Print button can be used to print out the optimisation results.

After the form was closed (“Done”) the arrow will jump to the next position, the begin of the pesticide optimisation (see Figure 18).

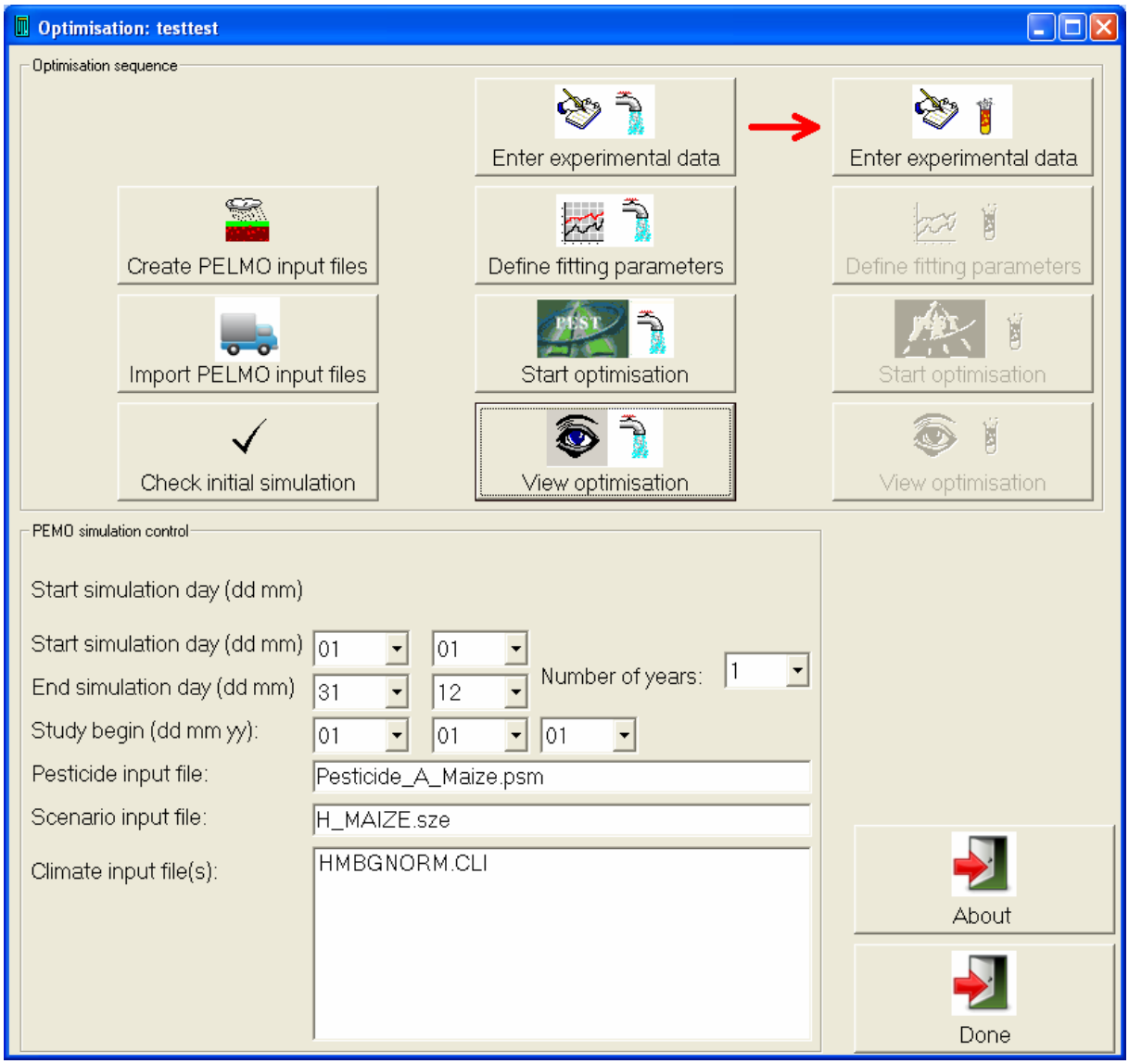

Figure 18: *InversePELMO*: *InversePELMO*: experimental data (pesticide fate)

4.4.8. Step 8: Enter experimental data (pesticide fate)

For the optimisation of the pesticide fate the experimental results has to be entered in a specific form (see Figure 19).

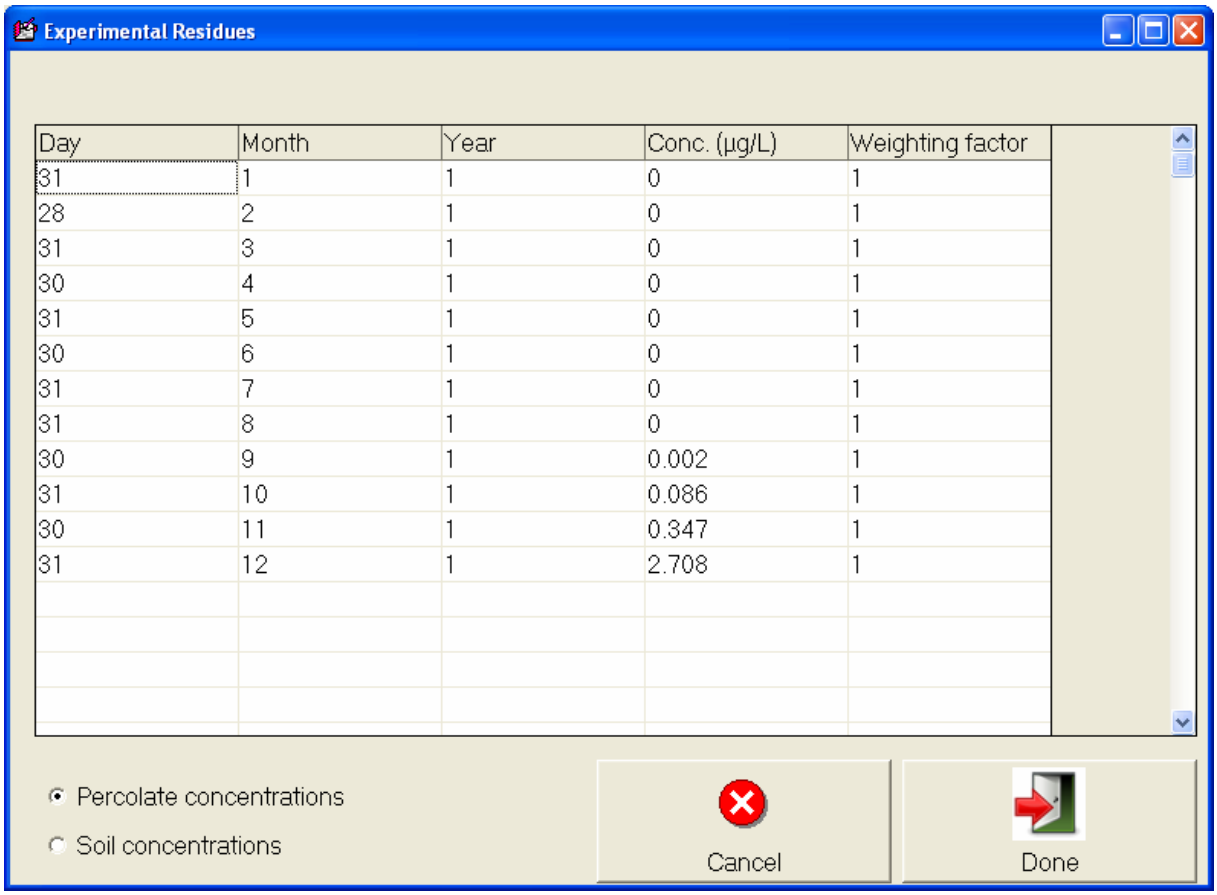

Figure 19: *InversePELMO*: Experimental concentrations in the percolate

Dependent on what input data is available (see the radio button on the form in Figure 19) either percolate concentrations or soil concentrations have to be entered.
If percolate concentrations should be used for the optimisation the concentration in µg/L are needed for each sampling date during the study. If appropriate the individual sampling could be characterised by weighting factors in the final column. The user cannot enter any date her, because the sampling dates are taken from the previous percolate optimisation.
If the user wants to use soil concentrations instead, the respective table is loaded when the radio button is used (Figure 20).

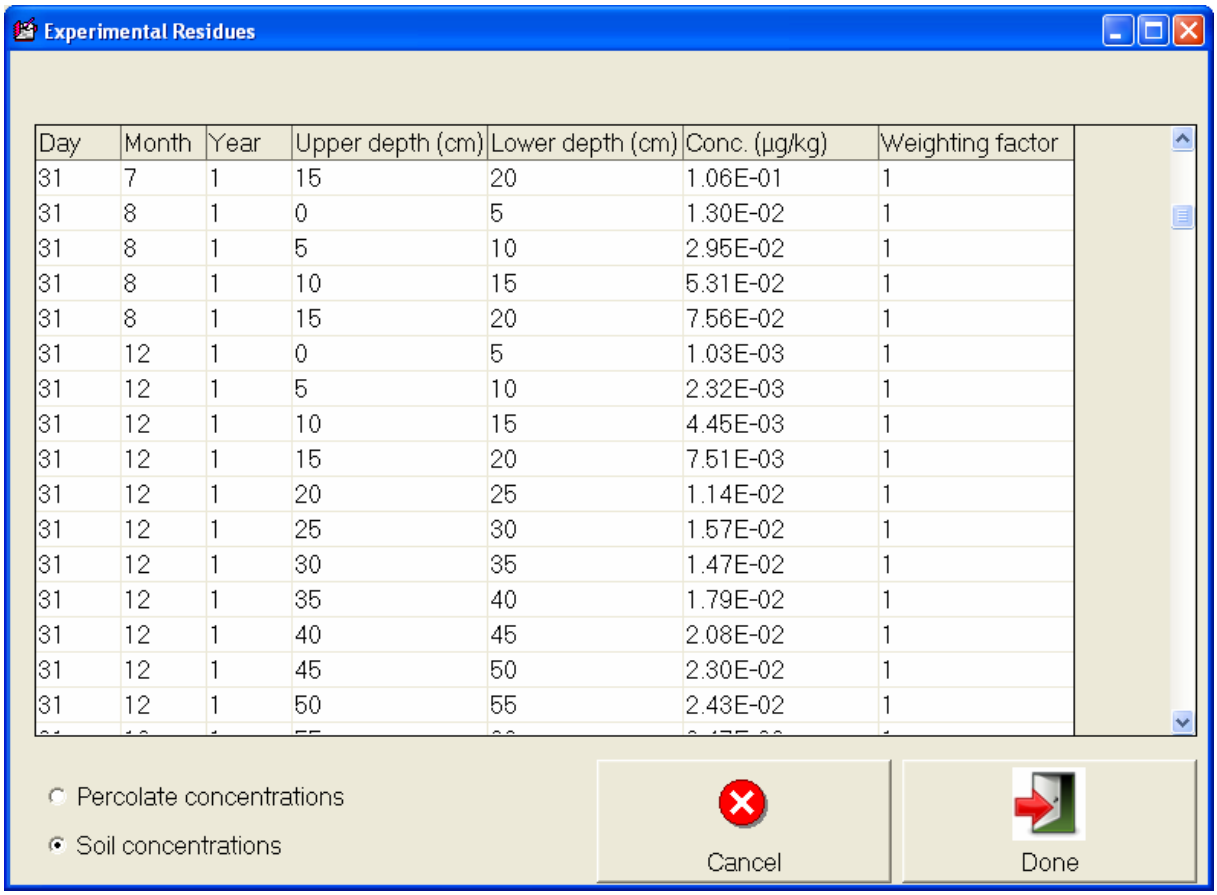

Figure 20: *InversePELMO*: Experimental soil concentrations

Soil concentrations have to be given in µg/kg together with the sampling date and the sampling depth.

For both tables it is not necessary to type all information the user can also paste them in as a table (e.g. from MS Excel or MS Word).

If the form has been filled correctly (e.g. no negative figures) it can be closed using the "Done" button and the arrow on the optimisation form will jump to the next button to enter all information about the input parameters used in the optimisation (see Figure 21)

Figure 21: *InversePELMO*: define fitting parameters for the hydrology in soil

4.4.9. Step 9: Enter fitting parameter (pesticide fate)

In step 9 the parameters used in the optimisation have to be characterised in a specific form (see Figure 22).

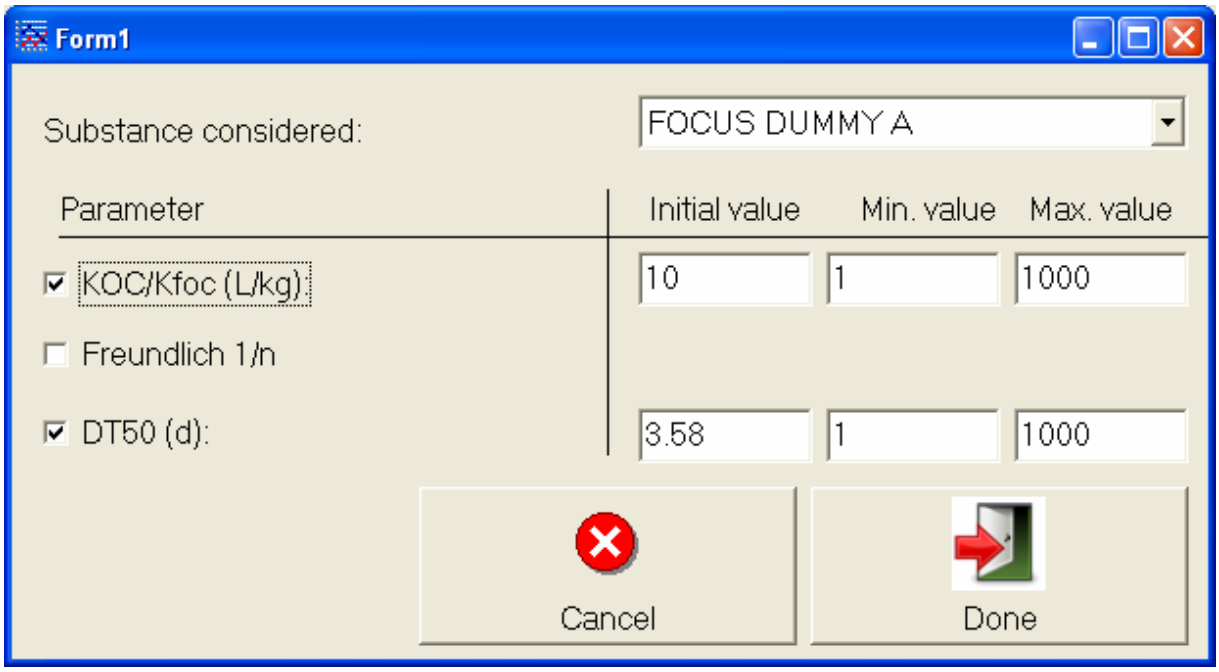

Figure 22: *InversePELMO*: Parameter for fitting pesticide fate

Three PELMO input parameters dominating pesticide fate in soil can be used to do the fitting.

- KOC/Kfoc: linear or non-linear sorption factor
- Freundlich 1/n Kc-factor (mid season): linear correction factor for daily potential evapotranpiration when the crop is growing
- DT50: Time to reach 50 % degradation in soil

If parameters shall be considered for the optimisation their initial values and their range have to be specified. If a parameter is not checked the respective input field is invisible.
As the DT50 in soil is not an input parameter in PELMO it will be converted into the respective rate constant (which is the actual input parameter) internally.
InversePELMO is able to analyse the fate of pesticides as well as of transformation products. If metabolites have been defined in the PSM-file previously, the user can select the compound using the list box on top of the form.
If the form has been filled correctly (e.g. no negative figures, no minimum values higher than maximum values) it can be closed using the “Done” button and the arrow on the optimisation form will jump to the next button which is the button for starting the optimisation (see Figure 23).

4.4.10. Step 10: Optimisation of the hydrology in soil (pesticide fate)

In step 10 of the sequence the pesticide fate is optimised. During the optimisation PEST will call PELMO several times. After PEST terminated the user has to confirm that the optimisation didn't quit with an obvious error conditions.

Figure 23: *InversePELMO*: start optimisation of the pesticide fate

Only after confirmation the arrow will move to the next button (see Figure 24).

4.4.11. Step 11: View the optimisation (pesticide fate)

In step 11 the user can evaluate the results of the fate optimisation.

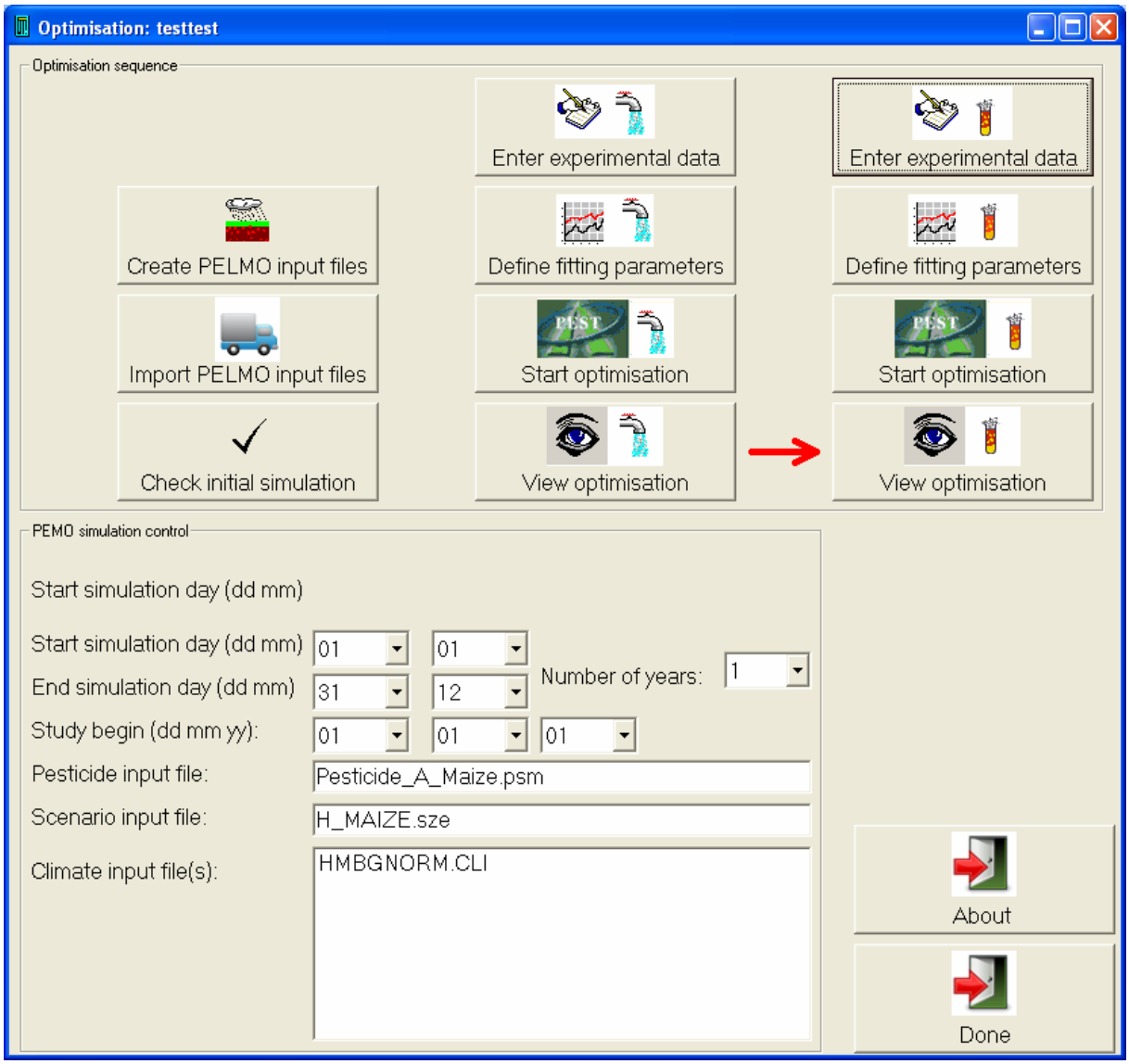

Figure 24: *InversePELMO*: Analyse the results of the optimisation for soil hydrology (percolate)

After clicking at the respective button (arrow on Figure 24) a form is loaded showing the experimental and optimised results graphically, either soil (Figure 25) or percolate concentrations (Figure 26). If soil concentrations are presented different diagrams are available for each soil layer. After a click with the left mouse button the next soil layer will be shown.

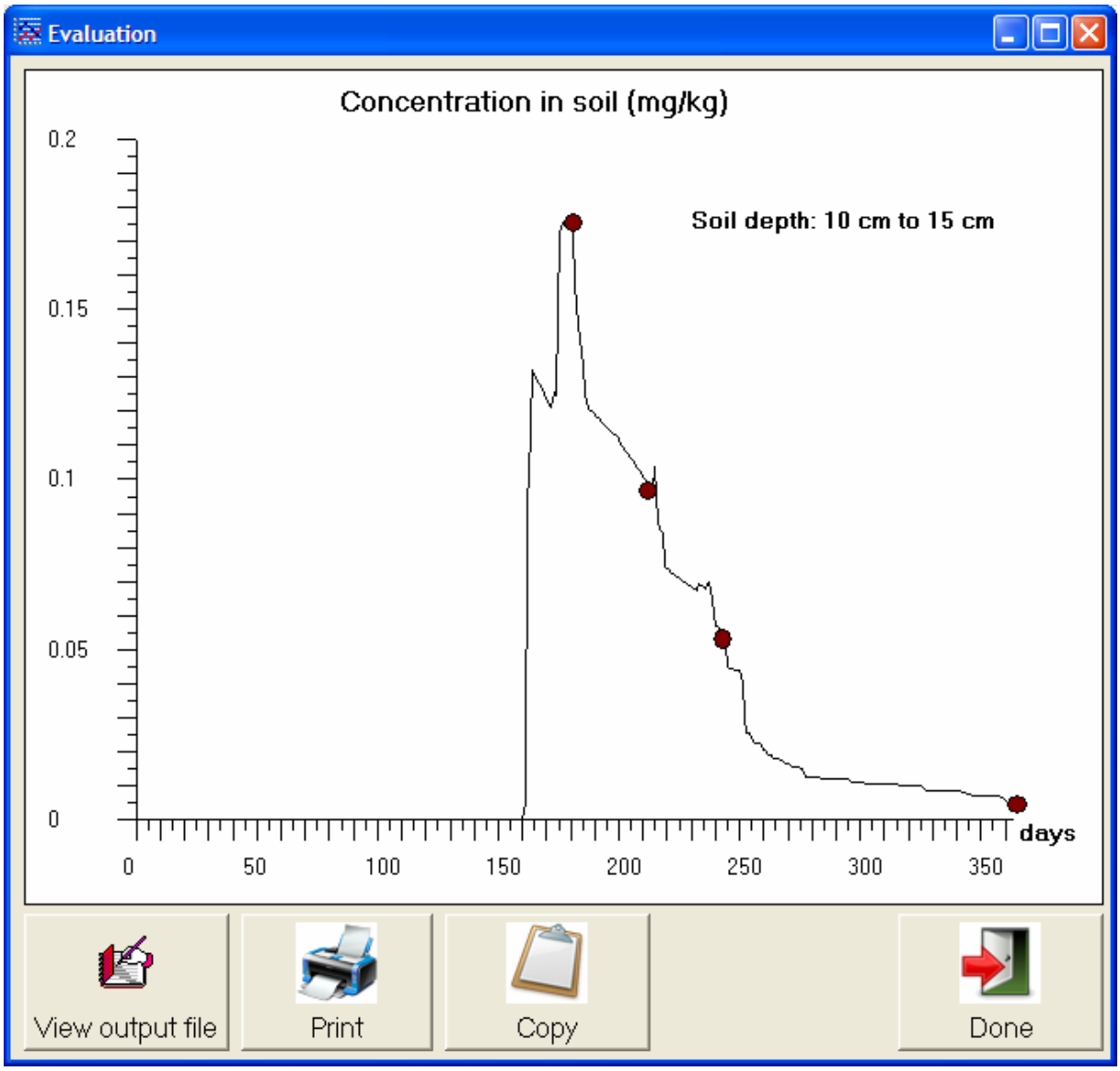

Figure 25: *InversePELMO*: View the results of the optimisation (soil concentrations)

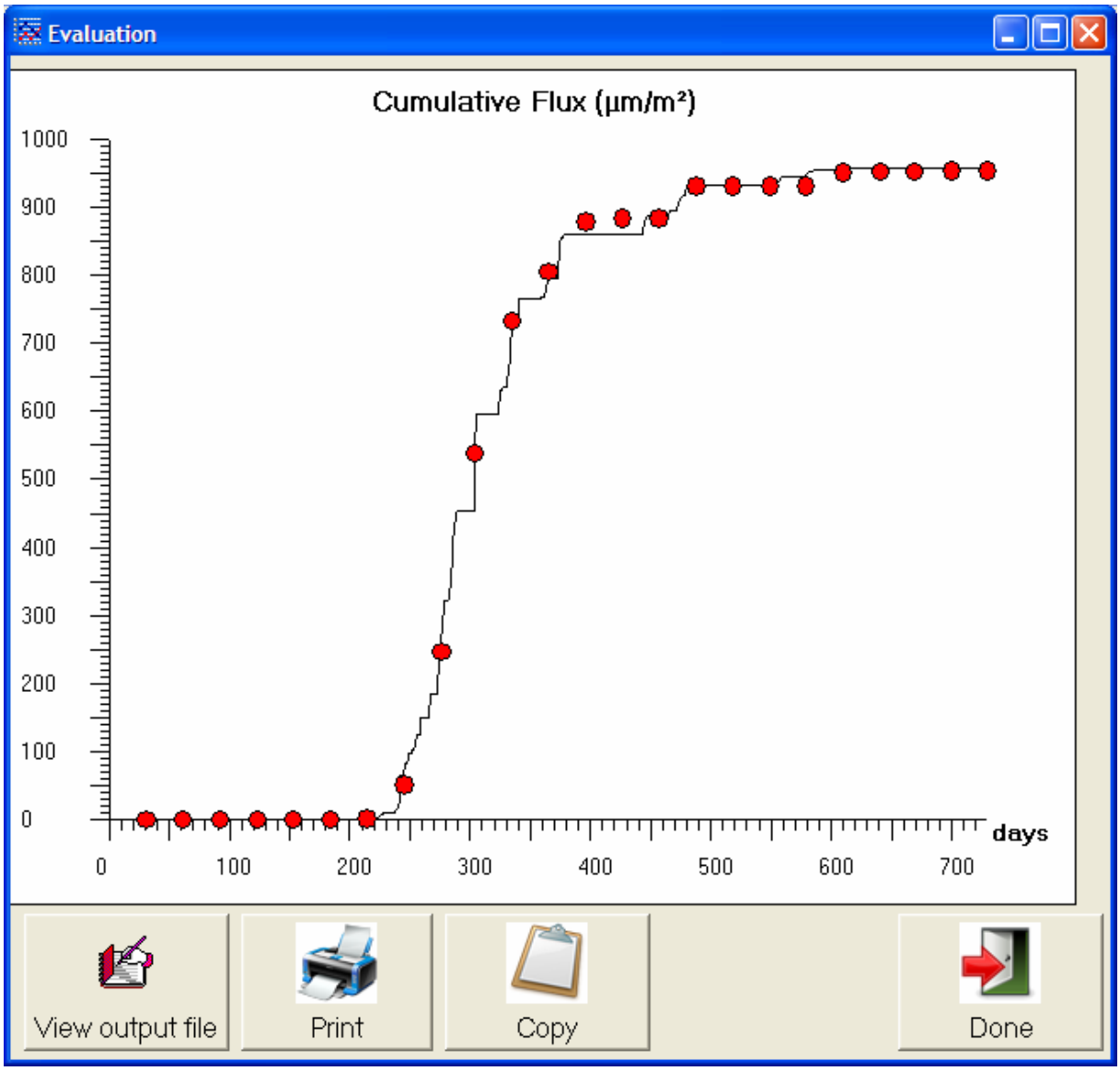

Figure 26: *InversePELMO*: View the results of the optimisation (cumulative flux)

The circles always represent the experimental data; the curve stands for the PELMO optimisation. Detailed output describing the optimisation procedure is available via the button “View output file” (Figure 27).

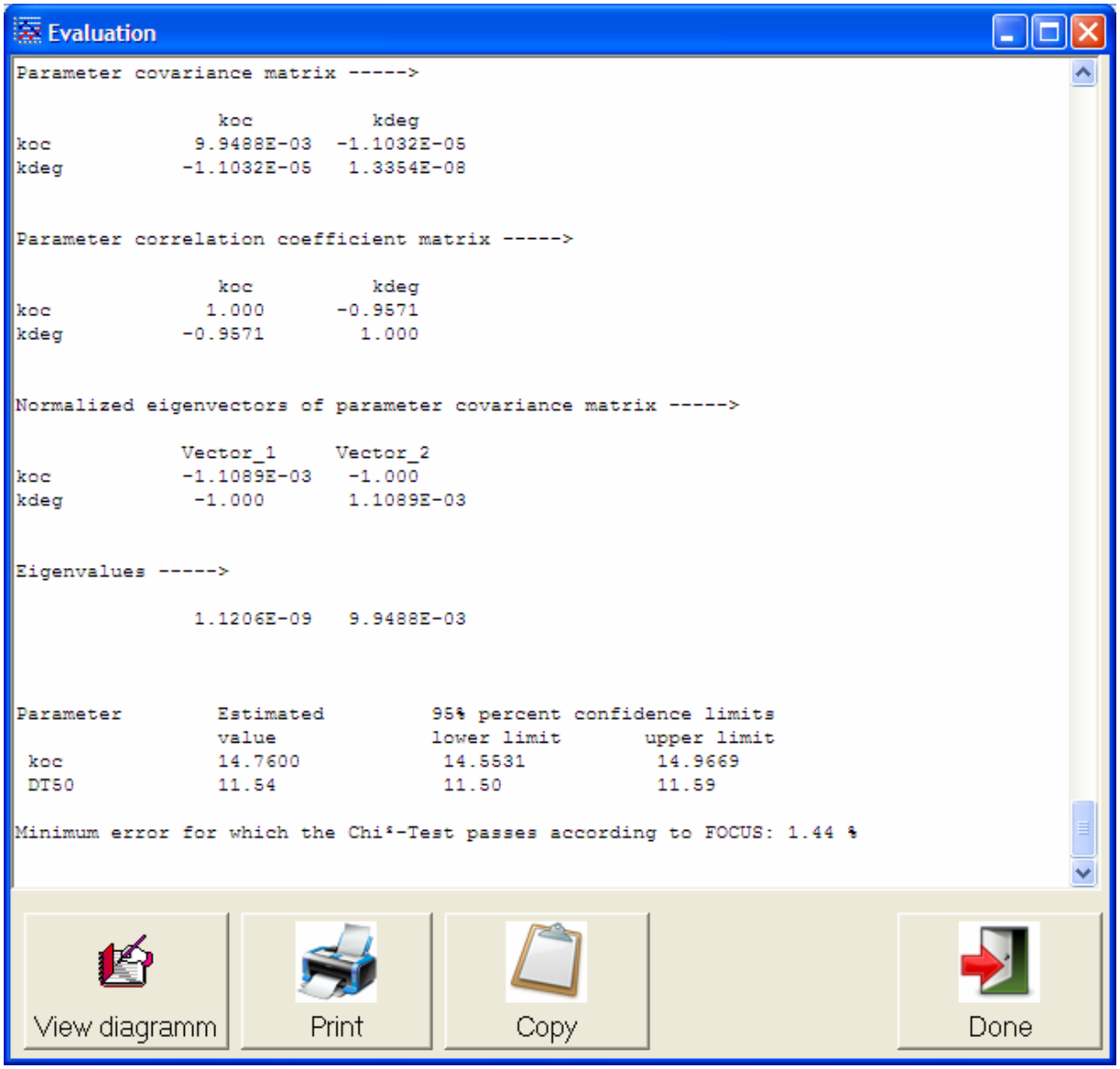

Figure 27: *InversePELMO*: Evaluate the results of the optimisation (pesticide fate)

The standard output file of PEST (extension “rec”) is used here, but with additional information included about the error at which the chi² test passes. The methodology is according to FOCUS degradation kinetics (FOCUS 2006).

As the DT50 in soil is not an input parameter in PELMO it has to be converted into the respective rate constant. Consequently, PEST will not give information about the optimisation for DT50 values. This information was therefore also added to the original PEST output file.

The copy button puts either graphic or the text into the clipboard, whereas the Print button can be used to print out the optimisation results.

5. Results of test simulations

In this chapter results of two different studies are used to check the inverse modelling abilities of *InversePELMO* and PEST.
Whereas the first case is a hypothetic example the second example is based on real lysimeter data.

5.1. Example data set 1: Leaching of Parent over a two years

5.1.1. Environmental data

For the soil data the standard Borstel soil was used with exactly the same description as given in the PELMO 3.0 soil data base. The soil profile information is summarised in Table 1.

Table 1: Borstel soil profile in the lysimeter (hypothetical test data set 1)

Horizon [cm]	0-30	30-57	57-73	73-90	90-110
Soil density [g/cm^3]	1.5	1.6	1.58	1.62	1.6
Sand [%]	68.3	67.0	96.2	98.8	100
Silt [%]	24.5	26.3	2.9	0.2	0
Clay [%]	7.2	6.7	0.9	0	0
OC [%]	1.5	1.0	0.2	0	0
initial soil water content [m³/m³]	0.05	0.05	0.05	0.05	0.05
Biodegradation factor [-]	1	0.16	0.09	0.13	0
pH-value	5.7	4.9	4.9	5.0	4.8

The Hamon equation was used to estimate potential evapotranspiration. The parameter linked to that process are summarised in the following table.

Table 2: Further input parameters influencing evapotranspiration (hypothetical test data set 1)

Parameter	Value
Minimum depth for evaporation (cm)	15
Kc0 (no crop)	1.0
Kc1 (mid season)	1.3
Kc2 (late season)	0.5

The crop considered for the simulation was maize with standard crop parameter setting.

For the climate during the lysimeter study the standard PELMO 3.0 climate files (Hamburg normal and wet weather) are used. The monthly and annual precipitation and temperature data is given in Table 3. Begin of the study 1 the 1st May.

Table 3: Climate data during the study (hypothetical test data set 1)

Month	Montly Precipitation [mm]	Annual Precipitation [mm]	Monthly Temperature [°C]	Annual Temperature [°C]
January	62.8		-0.25	
February	75.9		4.80	
March	69.8		6.09	
April	66.4		10.25	
May	80.4		10.45	
June	30.4		16.29	
July	142.6		15.23	
August	110.9		15.27	
September	25.8		15.78	
October	51.7		11.17	
November	55.5		4.37	
December	99.8		-0.75	
January	67.6		1.81	
February	18.3		-0.69	
March	93.7		4.95	
April	13.0	789.7	5.39	8.3
May	21.0		12.54	
June	94.5		15.55	
July	73.7		15.57	
August	72.9		15.74	
September	153.2		12.20	
October	52.9		10.45	
November	33.5		6.57	
December	83.2		-0.23	
January	62.8		-0.25	
February	75.9		4.80	
March	69.8		6.09	
April	66.4	859.8	10.25	9.1

5.1.2. Pesticide data

For the pesticide input data the example compound FOCUS B was considered, a fast leaching substance with KOC 17 L/kg of and DT50 of 20 d (Q10= 2.58).

The application pattern was a single application of 1 kg/ha to the soil surface on 1st May. An overview on all pesticide data is given in Table 4.

Table 4: Pesticide input parameters used for the test simulations

Parameter	Unit	Value
Molar mass	(g mol-1)	300
Solubility in water	(mg L-1)	90
Molar enthalpy of dissolution	(kJ mol-1)	27
Vapour pressure at 20° C	(mPa)	0.1
Molar enthalpy of vaporisation	(kJ mol-1)	95
Diffusion coefficient in water	(m2 d-1)	4.3 * 10-5
Gas diffusion coefficient	(m2 d-1)	0.43
Reference temperature for degradation, vaporisation and dissolution	(°C)	20
Reference soil moisture for degradation	(-)	at 10 kPa (field capacity)
Q10-factor (increase of degradation rate with an increase of temperature of 10°C)	(-)	2.58
Arrhenius activation energy	(kJ mol-1)	65.4
B (exponent of degradation - moisture relationship according to Walker)	(-)	0.7
Exponent of the FREUNDLICH-Isotherm	(-)	0.9
Non-equilibrium sorption	(-)	not considered
TSCF = transpiration stream concentration factor	(-)	0.5

5.1.3. Lysimeter results (hypothetical test data set 1)

The main results of the hypothetical study 1 are summarised in Table 5. The maximum concentration in the leachate was detected at the end of the first winter (February: 3.37 µg/L). The total percolate collected was 649.1 L/m².

Table 5: Percolate and percolate concentrations in the lysimeter (hypothetical test data set 1)

Month	Percolate (L/m²)	Concentration (µg/L)
May	0	0
June	0	0
July	0	0
August	0	0
September	5.6	0
October	27.36	0
November	18.22	0
December	66.42	0.022
January	62.36	0.378
February	62.63	1.399
March	46.75	2.193
April	25.93	2.265
May	27.11	2.075
June	0	1.95
July	19.43	1.792
August	40.37	1.336
September	0	0
October	0	0
November	16.98	0.934
December	93.98	0.454
January	56.67	0.143
February	9.68	0.087
March	69.61	0.053
April	0	0.034

5.1.4. Optimisation (hypothetical test data set 1)

For the optimisation of the percolate all possible parameters were considered in the fitting. Their initial values and their possible range are shown in Figure 28.

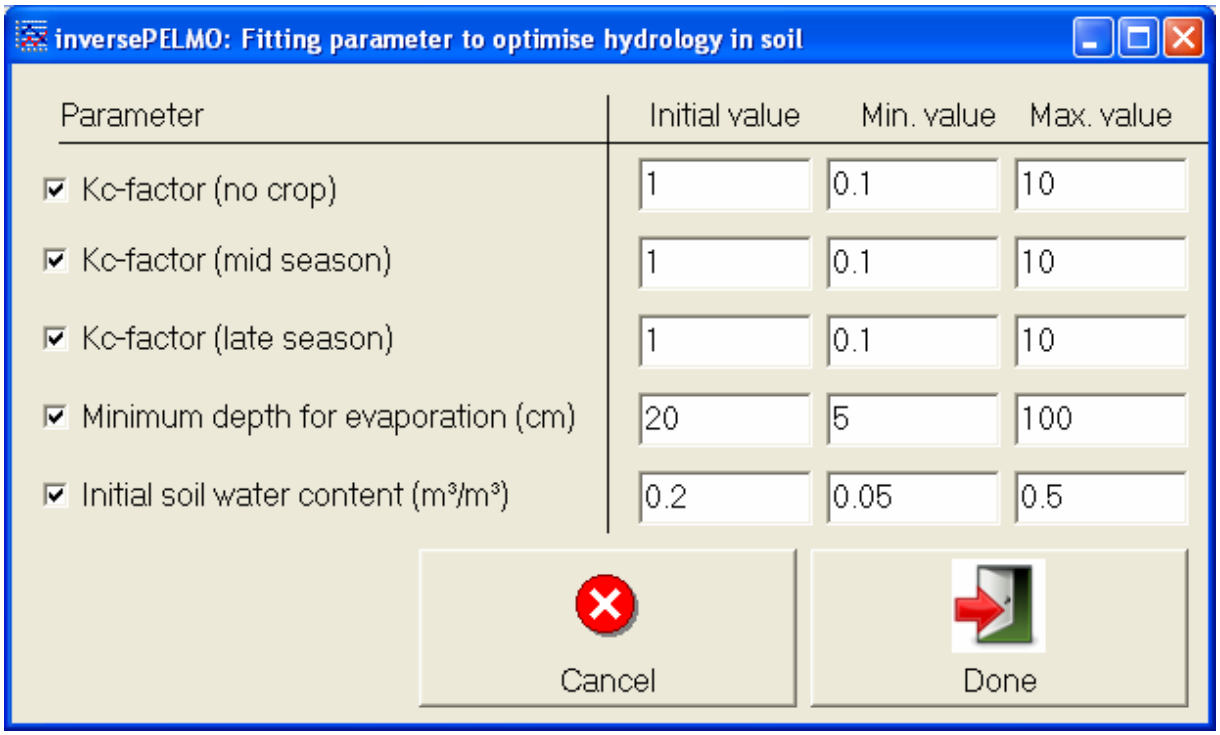

Figure 28: Parameters used in the optimisation of the percolate (hypothetical test data set 1)

After the optimisation the results summarised in Figure 29 were obtained.

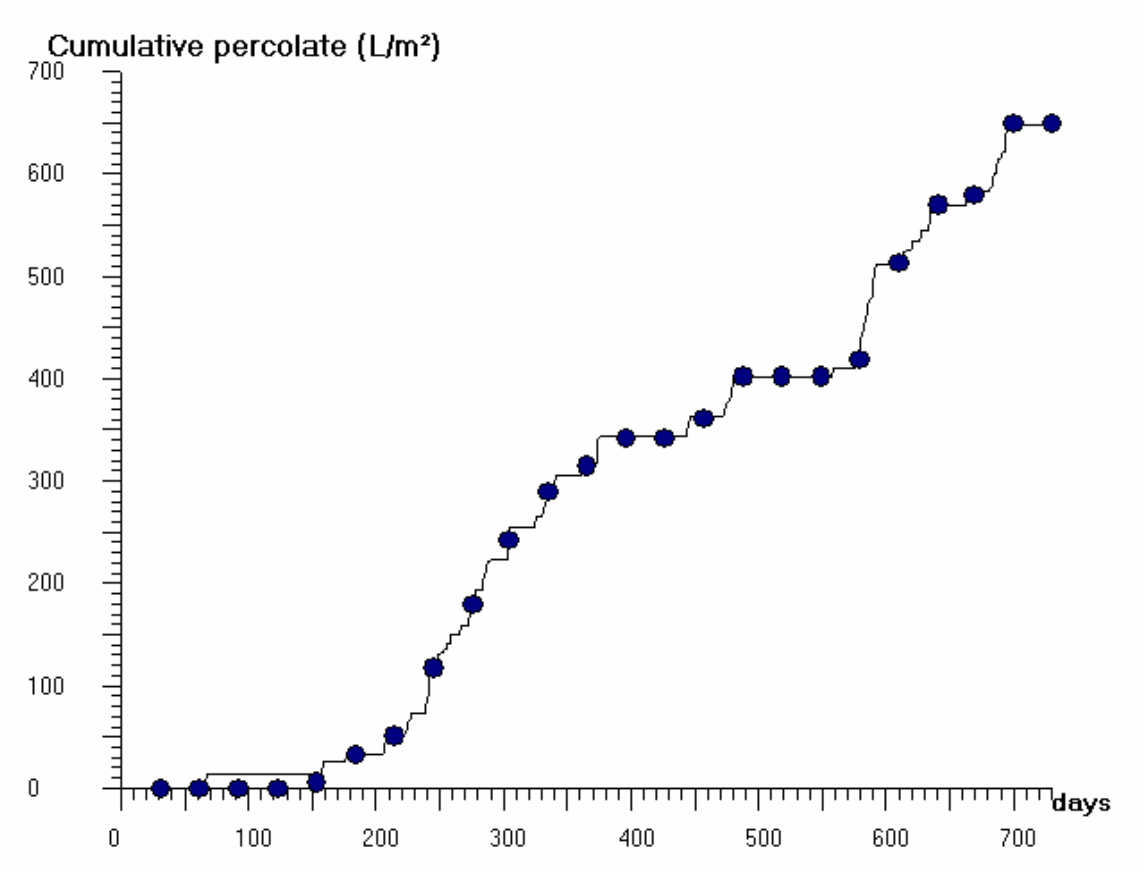

Figure 29: *R*esults of the optimisation (percolate, hypothetical test data set 1)

The minimum error for which the Chi²-Test passes according to FOCUS was found to be 1.28 % which supports the excellent agreement shown in the figure.

Table 6: Optimised parameter for the percolate (hypothetical test data set 1)

Parameter	Estimated value
KC0	0.98
KC1	1.34
KC2	4.07
ANETD	30
MOI0	0.2

The results summarised in Table 6 shows that the inverse modelling tool did not find the same parameter setting as used when producing the hypothetical test data. However, more important than identical parameters is the correct description of the percolate by the leaching model because many parameter combinations lead to similar results.

For the optimisation of the substance fluxes the parameters “DT50” and “KOC” were considered in the fitting. Their initial values and their possible range are shown in Figure 30.

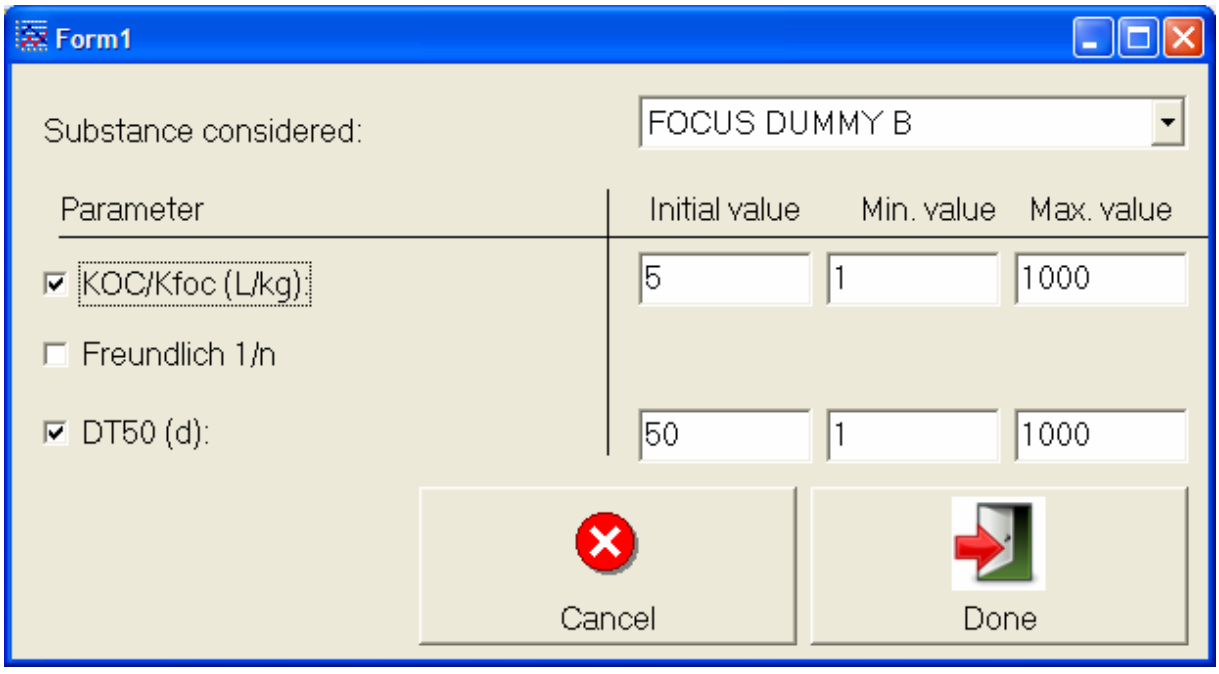

Figure 30: Parameters used in the optimisation of the substance flux (test data set 1)

After the optimisation the results summarised in Figure 31 were obtained.

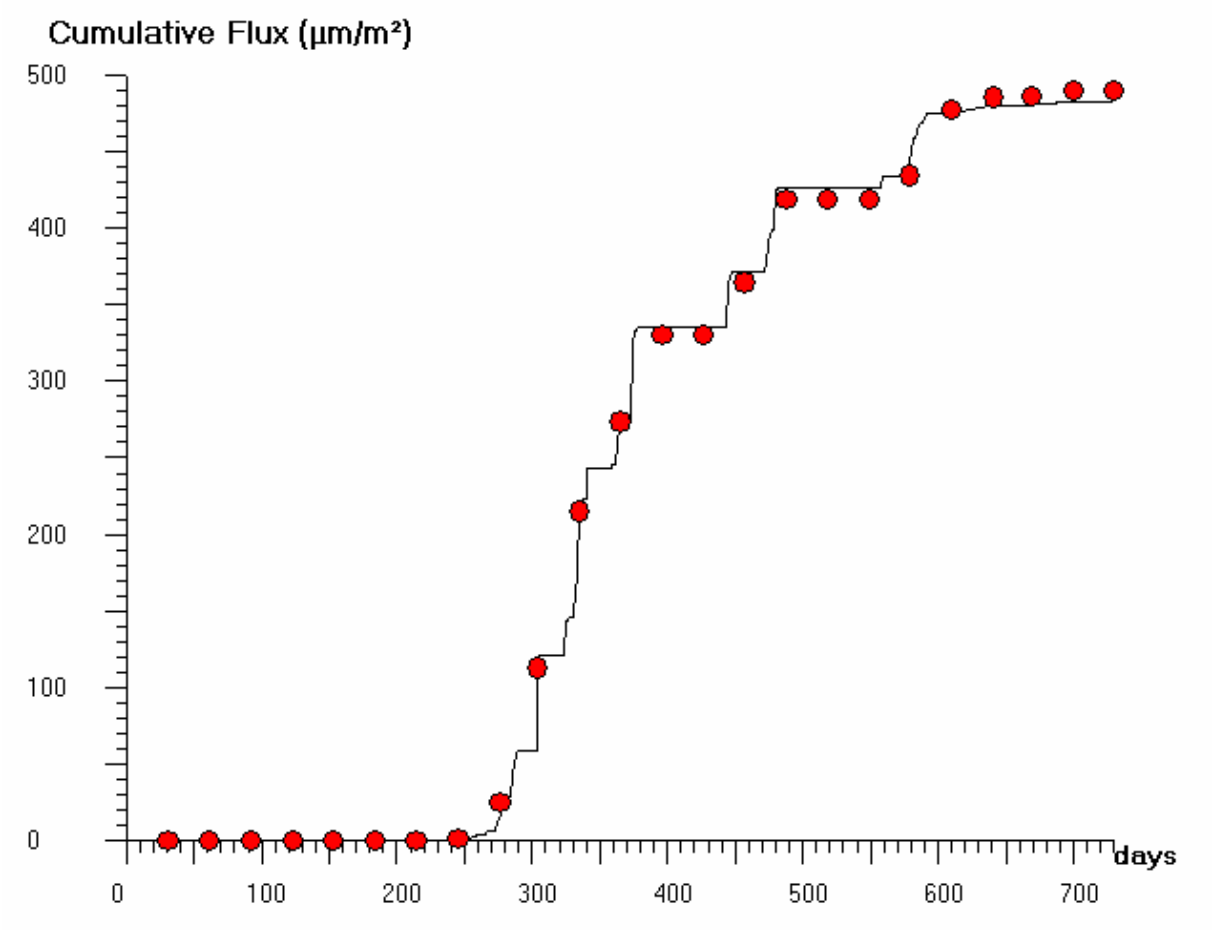

Figure 31: *R*esults of the optimisation (substance flux, hypothetical test data set 1)

The agreement is excellent as also expressed by the small FOCUS chi² error of 2.2 %.

Table 7: Optimised parameter for the substance fluxes (hypothetical test data set 1)

Parameter	Estimated value	95% confidence limits lower limit	95% confidence limits value	Original parameters
koc	13.570	13.29	13.570	17
DT50	12.82	12.77	12.82	20

Nevertheless, Table 7 shows that PEST did not find back the original parameter setting, but suggested different sorption and degradation data. Obviously, there are different combinations that lead to the same substance fluxes. PEST suggested a slightly lower koc and compensated the higher mobility by a shorter half life. But according to Figure 31 the alternative parameter combination leads to the same leaching behaviour in the study.

5.2. Test data set 2: Leaching of Parent over a 17 months

5.2.1. Environmental data

For the soil data the standard Borstel soil was used with exactly the same description as given in the PELMO 3.0 soil data base. The soil profile information is summarised in Table 1.

Table 8: Borstel soil profile in the lysimeter (test data set 2)

Horizon [cm]	0-30	30-57	57-73	73-90	90-110
Soil density [g/cm^3]	1.5	1.6	1.58	1.62	1.6
Sand [%]	68.3	67.0	96.2	98.8	100
Silt [%]	24.5	26.3	2.9	0.2	0
Clay [%]	7.2	6.7	0.9	0	0
OC [%]	1.5	1.0	0.2	0	0
initial soil water content [m³/m³]	0.05	0.05	0.05	0.05	0.05
Biodegradation factor [-]	1	0.5	0.3	0.3	0.3
pH-value	5.7	4.9	4.9	5.0	4.8

The Climatic conditions during the lysimeter study are summarised in Table 9, whereas the following two figures show the daily pattern.

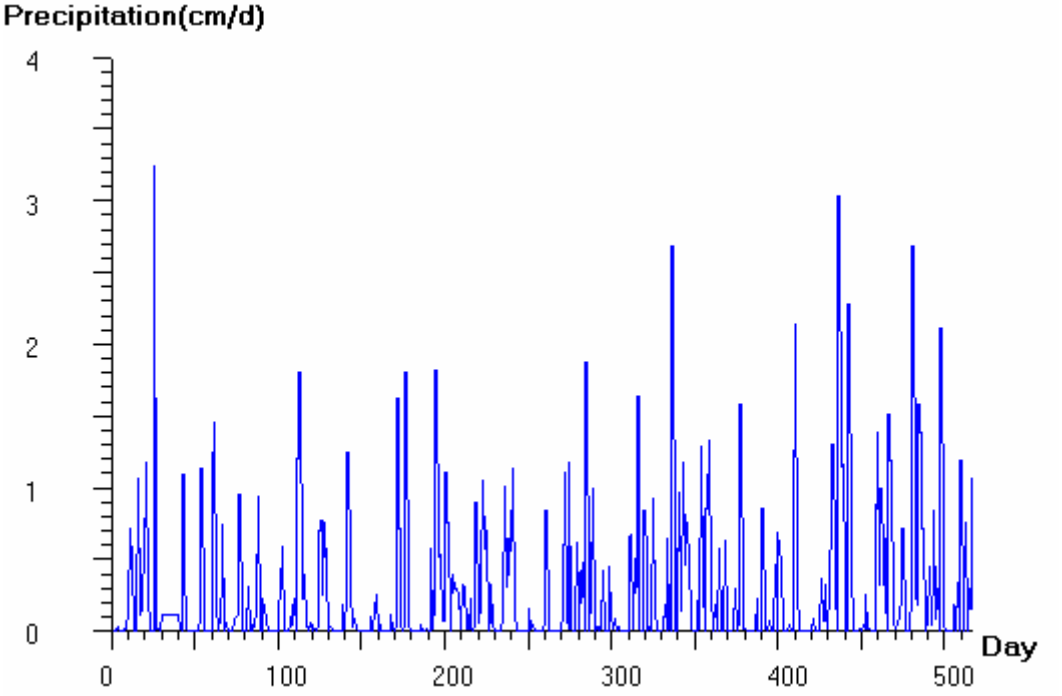

Figure 32: Daily precipitation at the lysimeter station from August 2008 to December 2009

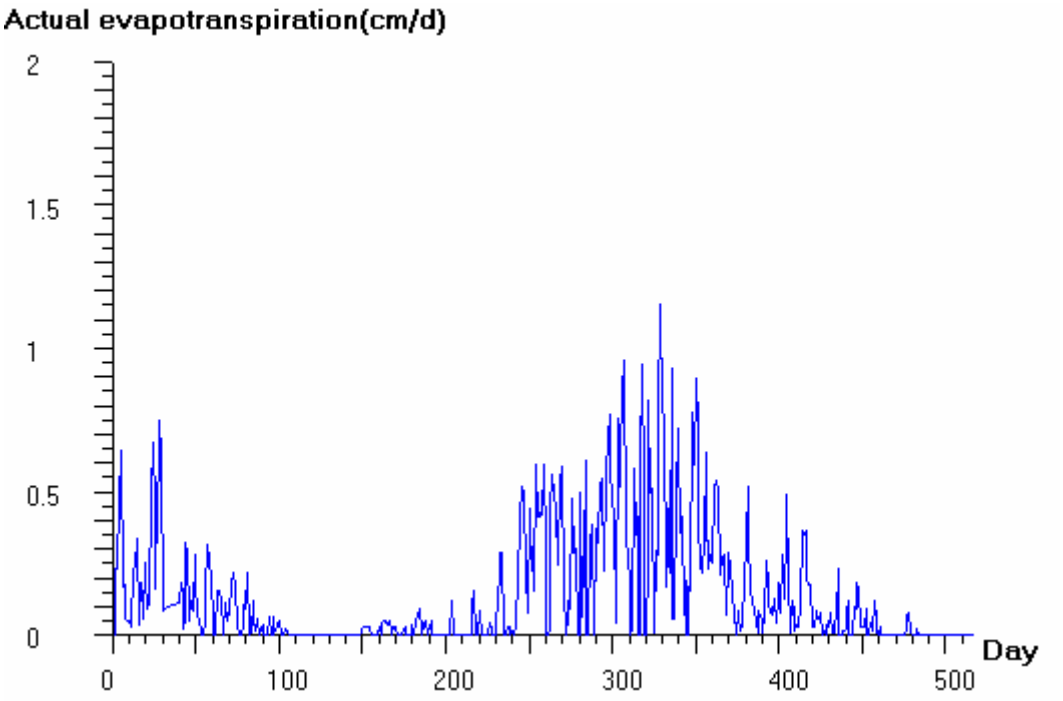

Figure 33: Actual ET at the lysimeter station from from August 2008 to December 2009

Table 9: Climate data during the study (test data set 2)

Month	Montly Precipitation [mm]	Annual Precipitation [mm]	Monthly PET* [mm]	Annual PET* [°C]	Monthly Temperature [°C]	Annual Temperature [°C]
August	87		105		13.9	
September	50		2		8.8	
October	60		20		7.9	
November	60		0		4.2	
December	56		1		0	
January	50		6		-2.6	
February	83		5		-1	
March	89		20		2.2	
April	25		3		10.7	
May	72		96		11.4	
June	65		3		12.3	
July	135	832	108	369	15.8	7.0
August	38		108		16.4	
September	64		2		12.6	
October	126		15		6.5	
November	159		0		5.8	
December	96	483	1	126	-1.4	8.0

* PET = potential evpotranspiration

The crop considered for the simulation was winter rape (two seasons) The standard crop and crop rotation information was used. Begin of the study 2 was the 1st August with an application of 1.2 kg/ha on 21st August.

5.2.2. Pesticide data

An overview on all pesticide data is given in Table 10.

Table 10: Pesticide input parameters used for the test simulations

Parameter	Unit	Value
Molar mass	(g mol-1)	100
Solubility in water	(mg L-1)	90
Molar enthalpy of dissolution	(kJ mol-1)	27
Vapour pressure at 20° C	(mPa)	0.1
Molar enthalpy of vaporisation	(kJ mol-1)	95
Diffusion coefficient in water	(m2 d-1)	4.3 * 10-5
Gas diffusion coefficient	(m2 d-1)	0.43
Reference temperature for degradation, vaporisation and dissolution	(°C)	20
Reference soil moisture for degradation	(-)	at 10 kPa (field capacity)
Q10-factor (increase of degradation rate with an increase of temperature of 10°C)	(-)	2.58
Arrhenius activation energy	(kJ mol-1)	65.4
B (exponent of degradation - moisture relationship according to Walker)	(-)	0.7
Exponent of the FREUNDLICH-Isotherm	(-)	0.9
Non-equilibrium sorption	(-)	not considered
TSCF = transpiration stream concentration factor	(-)	0.0

5.2.3. Lysimeter results (test data set 2)

The main results of the study 2 are summarised in Table 11. The maximum concentration in the leachate was detected at the end of the study (December: 0.55 µg/L). The total percolate collected was 767 L/m².

Table 11: Percolate and percolate concentrations in the lysimeter (test data set 2)

Month	Percolate (L/m²)	Concentration (µg/L)
August	47.9	0.00
October	76.7	0.00
November	52.75	0.00
December	45.05	0.00
January	33.1	0.00
February	91.4	0.00
August	148.35	0.00
October	87.65	0.14
November	93	0.45
December	91.25	0.55

5.2.4. Optimisation (test data set 2

For the optimisation of the percolate all possible parameters were considered in the fitting. Their initial values and their possible range are shown in Figure 28.

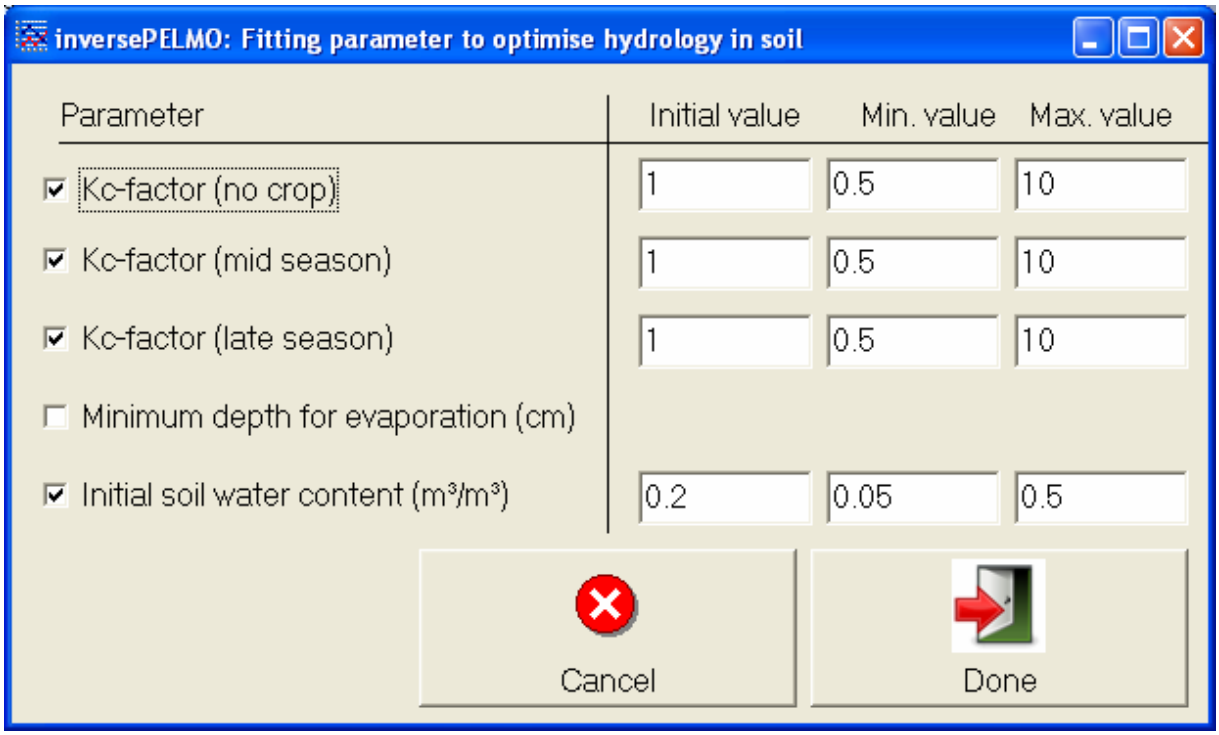

Figure 34: Parameters used in the optimisation of the percolate (test data set 2)

After the optimisation the results summarised in Figure 35 were obtained.

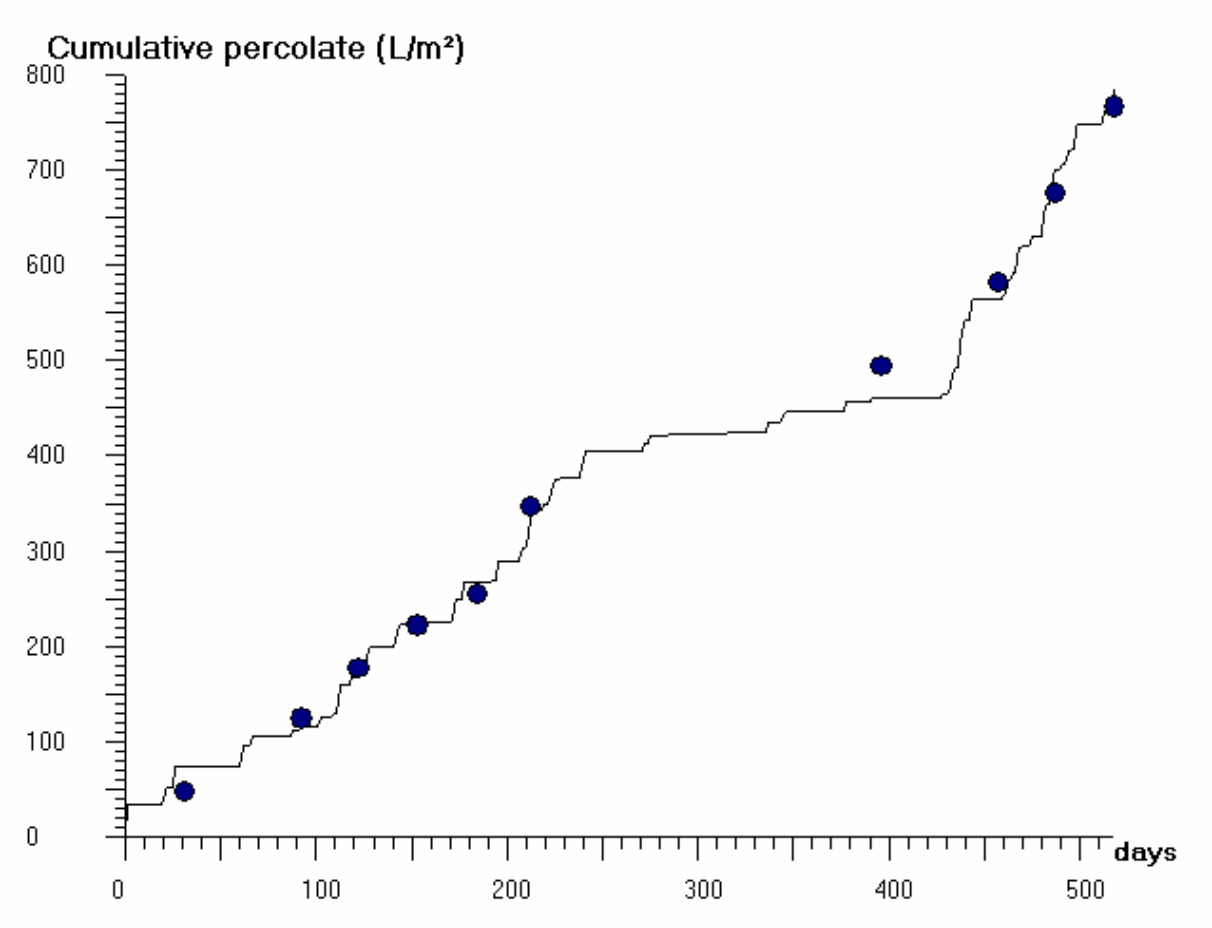

Figure 35: *R*esults of the optimisation (percolate, test data set 2)

The minimum error for which the Chi²-Test passes according to FOCUS was found to be 4.13 % which supports the excellent agreement shown in the figure.

Table 12: Optimised parameter for the percolate (test data set 2)

Parameter	Estimated value
KC0	0.5
KC1	2.304
KC2	1.00
MOI0	0.269

For the optimisation of the substance fluxes the parameters “DT50” and “KOC” were considered in the fitting. Their initial values and their possible range are shown in Figure 36.

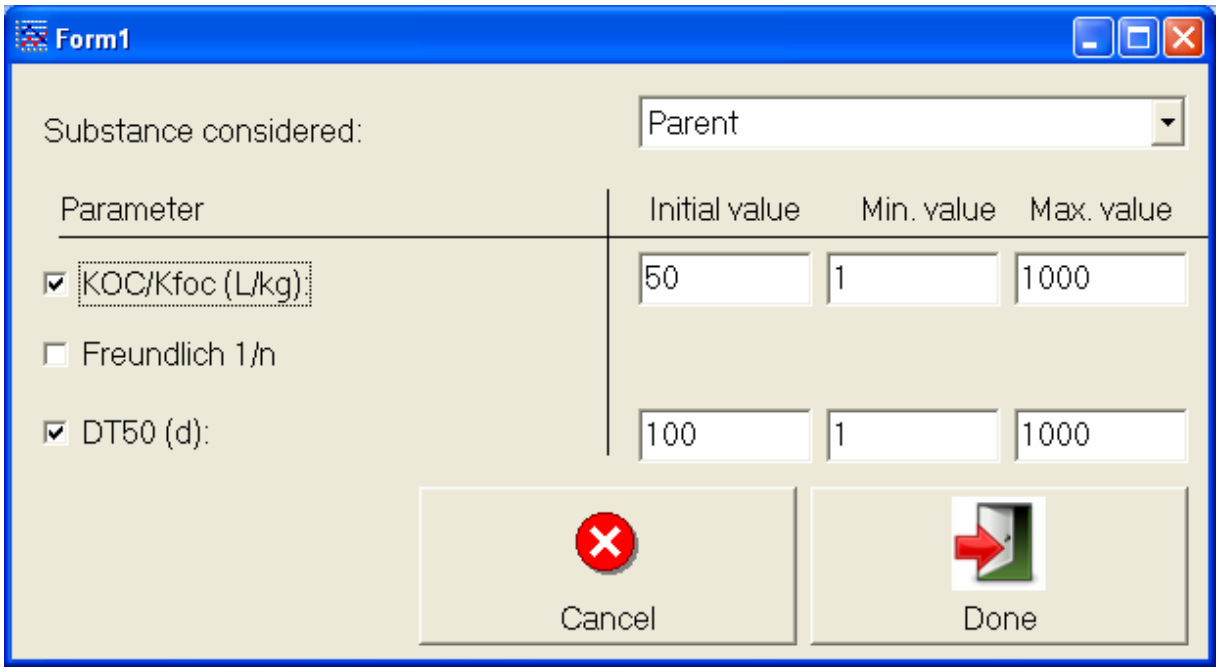

Figure 36: Parameters used in the optimisation of the substance flux (test data set 2)

After the optimisation the results summarised in Figure 37 were obtained.

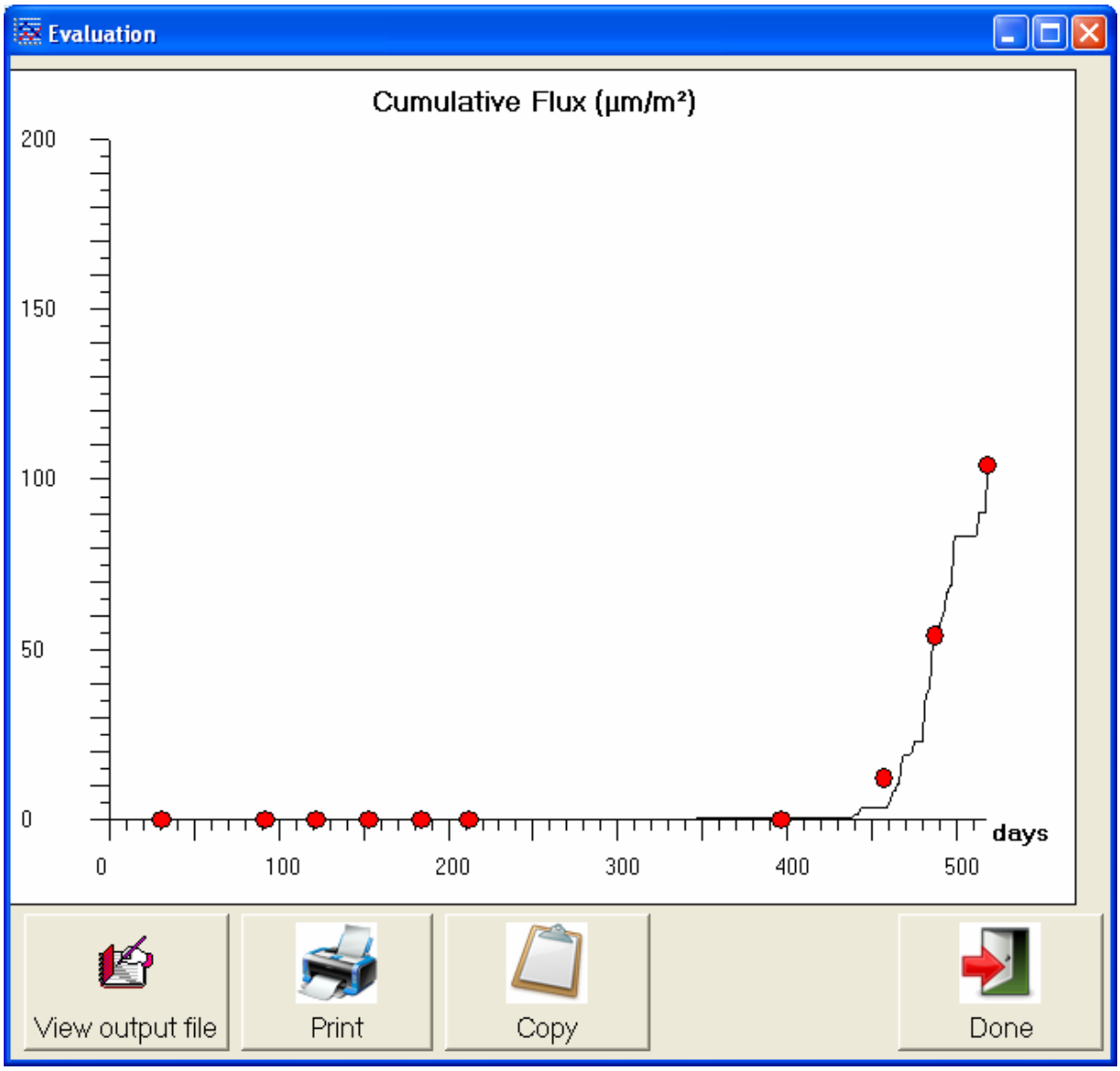

Figure 37: Results of the optimisation (substance flux, test data set 2)

The minimum error for which the Chi²-Test passes according to FOCUS was found to be 4.75 % which supports the excellent agreement shown in the figure.

Table 13: Optimised parameter for the substance fluxes (hypothetical test data set 2)

Parameter	Estimated value	95% confidence limits lower limit	value
koc	95.2	91.4	99.0
DT50	22.46	20.93	24.23

5.2.5. Hypothetical extension of the study (test data set 2

An interesting problem in connection with lysimeter studies is the question what would have been if the study had been extended. A prediction can be made based on the results of the inverse modelling studies as shown in the following example which uses the result of test data set 2 and assuming the same weather conditions as in the second year. The results are presented in Table 14.

Table 14: Extension of the lysimeter study (substance flux, hypothetical test data set 1*)

Month	Leachate (L/m²)	Concentration (µ/L)	Remark
August	69.14	0	
September	10.63	0	
October	40.94	0	
November	50.33	0	
December	50.59	0	
January	42.58	0	
February	67.16	0	
March	77.79	0.002	inverse modelling
April	0	0	study
May	10.8	0.006	
June	0	0	
July	31.93	0.017	
August	0	0	
September	13.82	0.028	
October	99.12	0.087	
November	145.7	0.316	
December	80.14	0.597	
January	53.46	0.75	
February	67.16	0.889	
March	77.79	0.991	
April	0	0	
May	10.8	0.956	
June	0	0	prediction
July	31.93	0.89	
August	0	0	
September	13.82	0.618	
October	99.12	0.424	
November	145.7	0.248	
December	80.14	0.18	

* optimised parameter setting

Based on the results of the previously performed inverse modelling study the PELMO calculation showed that the lysimeter study did not cover the peak maximum, instead the maximum peak is estimated to occur in March of the following year. The calculation furthermore showed that also in the next winter concentration above 0.1 µg/L can be expected.

5.2.6. Translation into standard conditions

The most interesting question usually is what concentrations can be considered if the lysimeter study had been performed under the official standard conditions. The results of the respective simulation (FOCUS Hamburg, 26 years of annual applications) are presented in Table 15.

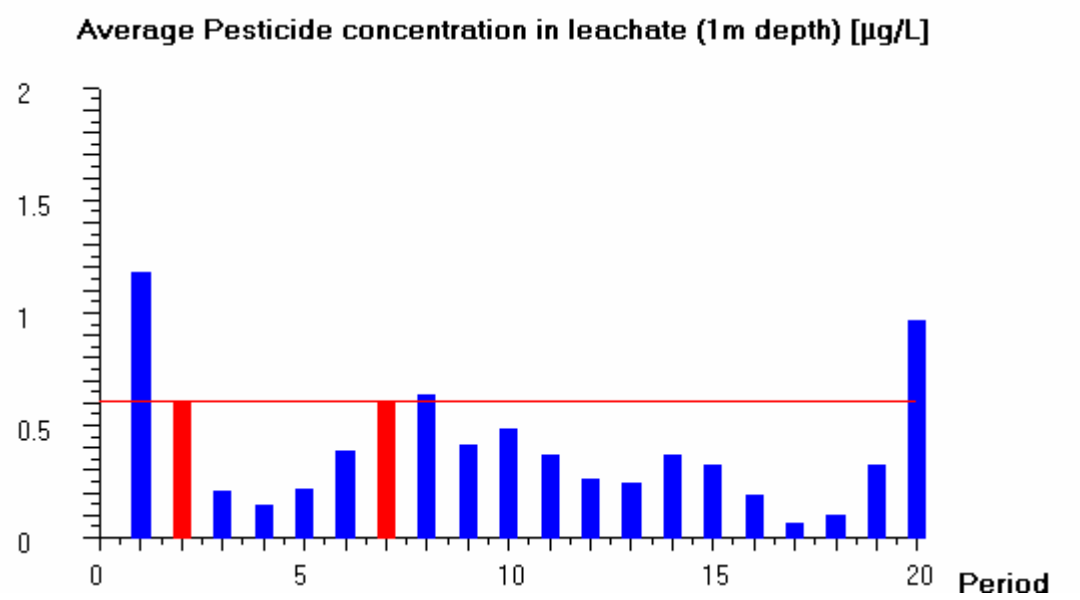

Figure 38: Results of the standard simulation with optimised parameters (FOCUS Hamburg)

Table 15: Pesticide in the percolate at 1 m soil depth* (FOCUS Hamburg)

Year	Pesticide Flux (g/ha)	Percolate (L/m^2)	Pesticide Conc. (µg/L)
1	3.47E-10	273.300	0.000
2	2.50E-07	78.8200	0.000
3	0.0215800	265.900	0.008
4	0.1968000	252.600	0.078
5	1.3630000	431.100	0.316
6	4.5400000	470.500	0.965
7	1.6590000	140.900	1.177
8	0.8473000	138.600	0.611
9	0.4894000	234.600	0.209
10	0.4048000	281.600	0.144
11	0.4784000	226.100	0.212
12	1.7700000	459.900	0.385
13	2.6330000	432.900	0.608
14	1.1830000	185.600	0.637
15	1.5250000	372.000	0.410
16	1.4950000	308.300	0.485
17	0.6419000	176.500	0.364
18	0.6015000	234.800	0.256
19	0.6459000	266.800	0.242
20	1.1640000	314.600	0.370
21	0.4984000	156.000	0.319
22	0.1471000	78.8200	0.187
23	0.1690000	265.900	0.064
24	0.2439000	252.600	0.097
25	1.3740000	431.100	0.319
26	4.5400000	470.500	0.965
Total	22.5106	5428.12	0.415
Perc.(8/13)	3.4803000	571.500	0.610

* annual applications of 1.2 kg/ha on 21st August 2011, optimised parameter setting

6. Discussion and Conclusions

The example simulations with all four test data set demonstrate that the link between *InversePELMO* and PELMO works sufficiently and results in adequate descriptions of what processes may have been occurred in lysimeter studies. Furthermore higher tier data on mobility and degradation can be obtained which can be used for refined modelling studies. With test simulations it was demonstrated that the results of inverse modelling studies with *InversePELMO* can also be used to transfer the lysimeter study to hypothetical situations such as

- extension of the study
- modification of the application pattern
- modification of crop data
- other climate scenarios

7. References

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8. Documentation of Model Output: *InversePELMO*

8.1. Example data set 1

8.1.1. Optimisation of soil hydrology

***InversePELMO* control file "sampling water.txt"**

```
01      05      01
 24
31      5       1       0       1
30      6       1       0       1
31      7       1       0       1
31      8       1       0       1
30      9       1       5.6     1
31      10      1       32.96   1
30      11      1       51.18   1
31      12      1       117.6   1
31      1       2       179.96  1
28      2       2       242.59  1
31      3       2       289.34  1
30      4       2       315.27  1
31      5       2       342.38  1
30      6       2       342.38  1
31      7       2       361.81  1
31      8       2       402.18  1
30      9       2       402.18  1
31      10      2       402.18  1
30      11      2       419.16  1
31      12      2       513.14  1
31      1       3       569.81  1
28      2       3       579.49  1
31      3       3       649.1   1
30      4       3       649.1   1
```

PEST control file “Pest_water.pst”

```
pcf
* control data
restart
   5  24   5  0
    1     1 single point
  5.0   2.0   0.3  0.03    10
  3.0   3.0 0.001
  0.1
   30  0.01     3     3  0.01     3
    1     1     1
* group definitions and derivative data
Kc0  relative 0.01  0.0  switch  2.0 parabolic
Kc1  relative 0.01  0.0  switch  2.0 parabolic
Kc2  relative 0.01  0.0  switch  2.0 parabolic
ANETD  relative 0.01  0.0  switch  2.0 parabolic
MOI0  relative 0.01  0.0  switch  2.0 parabolic
* parameter data
Kc0  none relative 0.5 0.1 10 Kc0       1.0000       0.00000
Kc1  none relative 0.5 0.1 10 Kc1       1.0000       0.00000
Kc2  none relative 0.5 0.1 10 Kc2       1.0000       0.00000
ANETD  none relative 30 5 100 ANETD       1.0000       0.00000
MOI0    none relative 0.2 0.01 0.5 MOI0       1.0000       0.00000
* observation data
o1    0                    1
o2    0                    1
o3    0                    1
o4    0                    1
o5    5.6                    1
o6    32.96                    1
o7    51.18                    1
o8    117.6                    1
o9    179.96                    1
o10    242.59                    1
o11    289.34                    1
o12    315.27                    1
o13    342.38                    1
o14    342.38                    1
o15    361.81                    1
o16    402.18                    1
o17    402.18                    1
o18    402.18                    1
o19    419.16                    1
o20    513.14                    1
o21    569.81                    1
o22    579.49                    1
o23    649.1                    1
o24    649.1                    1
* model command line
run_water
* model input/output
scenario.tpl  BORSTEL_Example_1.SZE
pest.ins pest_water.plm
* prior information
```

PELMO output file “PEST_water.plm”

```
0031 31 05 01  2.2205E-14
0061 30 06 01  4.57984E-14
0092 31 07 01  13.8470000000001
0123 31 08 01  13.8470000000001
0153 30 09 01  13.8470000000001
0184 31 10 01  32.6090000000001
0214 30 11 01  51.1211000000001
0245 31 12 01  117.7021
0276 31 01 02  180.24083
0304 28 02 02  243.13033
0335 31 03 02  290.329424
0365 30 04 02  317.046424
0396 31 05 02  344.161524
0426 30 06 02  344.161524
0457 31 07 02  362.501524
0488 31 08 02  402.136824
0518 30 09 02  402.136824
0549 31 10 02  402.136824
0579 30 11 02  417.461424
0610 31 12 02  511.514924
0641 31 01 03  568.392164
0669 28 02 03  578.281764
0700 31 03 03  648.351524
0730 30 04 03  648.351524
```

PEST output file “Pest_water.rec”

```
                PEST RUN RECORD: CASE PEST_PESTICIDE


PEST run mode:-

   Parameter estimation mode


Case dimensions:-

   Number of parameters                :    2
   Number of adjustable parameters     :    2
   Number of parameter groups          :    2
   Number of observations              :   24
   Number of prior estimates           :    0


Model command line(s):-

   run_pesticide


Jacobian command line:-

   na


Model interface files:-

   Templates:
      PESTICIDE.TPL
   for model input files:
      PESTICIDE_B_EXAMPLE_1.PSM

   (Parameter values written using single precision protocol.)
   (Decimal point always included.)

   Instruction files:
      PEST.INS
   for reading model output files:
      PEST_FLUX.PLM


PEST-to-model message file:-

   na


Derivatives calculation:-

Param        Increment   Increment   Increment   Forward or   Multiplier  Method
group        type                    low bound   central      (central)   (central)
koc          relative    1.0000E-02   none        switch        2.000     parabolic
kdeg         relative    1.0000E-02   none        switch        2.000     parabolic


Parameter definitions:-

Name         Trans-            Change       Initial        Lower          Upper
             formation         limit        value          bound          bound
koc          none              relative    5.00000        1.00000        1000.00
kdeg         none              relative   1.099000E-02   6.900000E-04   0.693150

Name         Group          Scale         Offset        Model command number
koc          koc           1.00000        0.00000            1
kdeg         kdeg          1.00000        0.00000            1


Prior information:-

   No prior information supplied


Observations:-
```

Observation name	Observation	Weight	Group
o1	0.00000	1.000	no_name
o2	0.00000	1.000	no_name
o3	0.00000	1.000	no_name
o4	0.00000	1.000	no_name
o5	0.00000	1.000	no_name
o6	0.00000	1.000	no_name
o7	0.00000	1.000	no_name
o8	1.46124	1.000	no_name
o9	25.0333	1.000	no_name
o10	112.653	1.000	no_name
o11	215.175	1.000	no_name
o12	273.907	1.000	no_name
o13	330.160	1.000	no_name
o14	330.160	1.000	no_name
o15	364.979	1.000	no_name
o16	418.913	1.000	no_name
o17	418.913	1.000	no_name
o18	418.913	1.000	no_name
o19	434.772	1.000	no_name
o20	477.439	1.000	no_name
o21	485.543	1.000	no_name
o22	486.385	1.000	no_name
o23	490.075	1.000	no_name
o24	490.075	1.000	no_name

Control settings:-

Initial lambda	: 5.0000
Lambda adjustment factor	: 2.0000
Sufficient new/old phi ratio per optimisation iteration	: 0.30000
Limiting relative phi reduction between lambdas	: 3.00000E-02
Maximum trial lambdas per iteration	: 10
Maximum factor parameter change (factor-limited changes)	: na
Maximum relative parameter change (relative-limited changes)	: 3.0000
Fraction of initial parameter values used in computing change limit for near-zero parameters	: 1.00000E-03
Allow bending of parameter upgrade vector	: no
Allow parameters to stick to their bounds	: no
Relative phi reduction below which to begin use of central derivatives	: 0.10000
Relative phi reduction indicating convergence	: 0.10000E-01
Number of phi values required within this range	: 3
Maximum number of consecutive failures to lower phi	: 3
Minimal relative parameter change indicating convergence	: 0.10000E-01
Number of consecutive iterations with minimal param change	: 3
Maximum number of optimisation iterations	: 30
Attempt automatic user intervention	: no

OPTIMISATION RECORD

INITIAL CONDITIONS:
Sum of squared weighted residuals (ie phi) = 6.10098E+05

Current parameter values
koc 5.00000
kdeg 1.099000E-02

OPTIMISATION ITERATION NO. : 1
Model calls so far : 1
Starting phi for this iteration: 6.10098E+05

Lambda = 5.0000 ----->
Phi = 1.65784E+05 (0.272 of starting phi)

No more lambdas: phi is less than 0.3000 of starting phi
Lowest phi this iteration: 1.65784E+05

Current parameter values		Previous parameter values	
koc	5.00600	koc	5.00000
kdeg	1.560000E-02	kdeg	1.099000E-02

Maximum relative change: 0.4195 ["kdeg"]

```
OPTIMISATION ITERATION NO.        :    2
   Model calls so far             :    4
   Starting phi for this iteration:  1.65784E+05

       Lambda =   2.5000     ----->
          Phi =  1.56340E+05  (  0.943 of starting phi)

       Lambda =   1.2500     ----->
          Phi =  1.55900E+05  (  0.940 of starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:  1.55900E+05
   Relative phi reduction between optimisation iterations less than 0.1000
   Switch to central derivatives calculation

      Current parameter values                Previous parameter values
      koc              5.04200                koc              5.00600
      kdeg            1.671000E-02            kdeg            1.560000E-02
   Maximum relative change: 7.1154E-02 ["kdeg"]


OPTIMISATION ITERATION NO.        :    3
   Model calls so far             :    8
   Starting phi for this iteration:  1.55900E+05

       Lambda =  0.62500     ----->
          Phi =  9.59417E+05  (  6.154 times starting phi)

       Lambda =  0.31250     ----->
          Phi =  1.60826E+06  ( 10.316 times starting phi)

       Lambda =   1.2500     ----->
          Phi =  1.80902E+05  (  1.160 times starting phi)

       Lambda =   2.5000     ----->
          Phi =  1.33430E+05  (  0.856 of starting phi)

       Lambda =   5.0000     ----->
          Phi =  1.51729E+05  (  0.973 of starting phi)

   No more lambdas: phi rising
   Lowest phi this iteration:  1.33430E+05

      Current parameter values                Previous parameter values
      koc              6.01900                koc              5.04200
      kdeg            2.063000E-02            kdeg            1.671000E-02
   Maximum relative change: 0.2346     ["kdeg"]


OPTIMISATION ITERATION NO.        :    4
   Model calls so far             :   17
   Starting phi for this iteration:  1.33430E+05

       Lambda =   2.5000     ----->
          Phi =  1.31355E+05  (  0.984 of starting phi)

       Lambda =   1.2500     ----->
          Phi =  1.30446E+05  (  0.978 of starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:  1.30446E+05

      Current parameter values                Previous parameter values
      koc              6.10300                koc              6.01900
      kdeg            2.147000E-02            kdeg            2.063000E-02
   Maximum relative change: 4.0717E-02 ["kdeg"]


OPTIMISATION ITERATION NO.        :    5
   Model calls so far             :   23
   Starting phi for this iteration:  1.30446E+05

       Lambda =  0.62500     ----->
          Phi =  1.19313E+05  (  0.915 of starting phi)

       Lambda =  0.31250     ----->
          Phi =   91098.      (  0.698 of starting phi)

       Lambda =  0.15625     ----->
          Phi =  2.56993E+05  (  1.970 times starting phi)
```

```
   No more lambdas: phi rising
   Lowest phi this iteration:   91098.

      Current parameter values                Previous parameter values
      koc              7.81500                koc               6.10300
      kdeg           2.668000E-02             kdeg            2.147000E-02
   Maximum relative change: 0.2805     ["koc"]


OPTIMISATION ITERATION NO.        :    6
   Model calls so far             :   30
   Starting phi for this iteration:   91098.

       Lambda =  0.15625     ----->
          Phi =  1.92513E+05  (  2.113 times starting phi)

       Lambda =  7.81250E-02 ----->
          Phi =  4.90305E+05  (  5.382 times starting phi)

       Lambda =  0.31250     ----->
          Phi =   47871.      (  0.525 of starting phi)

       Lambda =  0.62500     ----->
          Phi =   72670.      (  0.798 of starting phi)

   No more lambdas: phi rising
   Lowest phi this iteration:   47871.

      Current parameter values                Previous parameter values
      koc              10.2400                koc               7.81500
      kdeg           3.122000E-02             kdeg            2.668000E-02
   Maximum relative change: 0.3103     ["koc"]


OPTIMISATION ITERATION NO.        :    7
   Model calls so far             :   38
   Starting phi for this iteration:   47871.

       Lambda =  0.31250     ----->
          Phi =   15984.      (  0.334 of starting phi)

       Lambda =  0.15625     ----->
          Phi =   19112.      (  0.399 of starting phi)

       Lambda =  0.62500     ----->
          Phi =   29252.      (  0.611 of starting phi)

   No more lambdas: phi rising
   Lowest phi this iteration:   15984.

      Current parameter values                Previous parameter values
      koc              12.1100                koc               10.2400
      kdeg           3.225000E-02             kdeg            3.122000E-02
   Maximum relative change: 0.1826     ["koc"]


OPTIMISATION ITERATION NO.        :    8
   Model calls so far             :   45
   Starting phi for this iteration:   15984.

       Lambda =  0.31250     ----->
          Phi =   11485.      (  0.719 of starting phi)

       Lambda =  0.15625     ----->
          Phi =   12288.      (  0.769 of starting phi)

       Lambda =  0.62500     ----->
          Phi =   9905.7      (  0.620 of starting phi)

       Lambda =   1.2500     ----->
          Phi =   6987.3      (  0.437 of starting phi)

       Lambda =   2.5000     ----->
          Phi =   2734.8      (  0.171 of starting phi)

   No more lambdas: phi is less than 0.3000 of starting phi
   Lowest phi this iteration:   2734.8

      Current parameter values                Previous parameter values
      koc              14.4200                koc               12.1100
      kdeg           3.334000E-02             kdeg            3.225000E-02
```

```
   Maximum relative change: 0.1908     ["koc"]


OPTIMISATION ITERATION NO.        :    9
   Model calls so far             :   54
   Starting phi for this iteration:   2734.8

       Lambda =   2.5000     ----->
          Phi =   478.67      (  0.175 of starting phi)

   No more lambdas: phi is less than 0.3000 of starting phi
   Lowest phi this iteration:   478.67

      Current parameter values                Previous parameter values
      koc              14.5200                koc               14.4200
      kdeg            3.300000E-02            kdeg             3.334000E-02
   Maximum relative change: 1.0198E-02 ["kdeg"]


OPTIMISATION ITERATION NO.        :   10
   Model calls so far             :   59
   Starting phi for this iteration:   478.67

       Lambda =   1.2500     ----->
          Phi =   309.72      (  0.647 of starting phi)

       Lambda =  0.62500     ----->
          Phi =   300.94      (  0.629 of starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:   300.94

      Current parameter values                Previous parameter values
      koc              14.7800                koc               14.5200
      kdeg            3.305000E-02            kdeg             3.300000E-02
   Maximum relative change: 1.7906E-02 ["koc"]


OPTIMISATION ITERATION NO.        :   11
   Model calls so far             :   65
   Starting phi for this iteration:   300.94

       Lambda =  0.31250     ----->
          Phi =   296.85      (  0.986 of starting phi)

       Lambda =  0.15625     ----->
          Phi =   296.85      (  0.986 of starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:   296.85

      Current parameter values                Previous parameter values
      koc              14.7900                koc               14.7800
      kdeg            3.304000E-02            kdeg             3.305000E-02
   Maximum relative change: 6.7659E-04 ["koc"]


OPTIMISATION ITERATION NO.        :   12
   Model calls so far             :   71
   Starting phi for this iteration:   296.85

       Lambda =  0.15625     ----->
          Phi =   296.85      (  1.000 times starting phi)

       Lambda =  7.81250E-02 ----->
          Phi =   296.85      (  1.000 times starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:   296.85

      Current parameter values                Previous parameter values
      koc              14.7900                koc               14.7900
      kdeg            3.304000E-02            kdeg             3.304000E-02
   Maximum relative change:  0.000     ["koc"]


OPTIMISATION ITERATION NO.        :   13
   Model calls so far             :   75
   Starting phi for this iteration:   296.85

       Lambda =  7.81250E-02 ----->
          Phi =   296.85      (  1.000 times starting phi)
```

```
      Lambda =  3.90625E-02 ----->
         Phi =   296.85      (  1.000 times starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:   296.85

      Current parameter values                Previous parameter values
      koc              14.7900                koc              14.7900
      kdeg            3.304000E-02            kdeg            3.304000E-02
   Maximum relative change:  0.000     ["koc"]

   Optimisation complete: relative parameter change less than 1.0000E-02
                          over  3 successive iterations.
   Total model calls:   79

   The model has been run one final time using best parameters.
   Thus all model input files contain best parameter values, and model
   output files contain model results based on these parameters.
```

OPTIMISATION RESULTS

Parameters ----->

Parameter	Estimated value	95% percent confidence limits lower limit	upper limit
koc	14.7900	14.6360	14.9440
kdeg	3.304000E-02	3.298439E-02	3.309561E-02

Note: confidence limits provide only an indication of parameter uncertainty.
They rely on a linearity assumption which may not extend as far in parameter space as the confidence limits themselves - see PEST manual.

See file PEST_PESTICIDE.SEN for parameter sensitivities.

Observations ----->

Observation	Measured value	Calculated value	Residual	Weight	Group
o1	0.00000	0.00000	0.00000	1.000	no_name
o2	0.00000	0.00000	0.00000	1.000	no_name
o3	0.00000	0.00000	0.00000	1.000	no_name
o4	0.00000	0.00000	0.00000	1.000	no_name
o5	0.00000	0.00000	0.00000	1.000	no_name
o6	0.00000	1.912200E-06	-1.912200E-06	1.000	no_name
o7	0.00000	1.061063E-04	-1.061063E-04	1.000	no_name
o8	1.46124	0.517289	0.943951	1.000	no_name
o9	25.0333	17.4226	7.61074	1.000	no_name
o10	112.653	101.647	11.0053	1.000	no_name
o11	215.175	210.598	4.57728	1.000	no_name
o12	273.907	274.922	-1.01527	1.000	no_name
o13	330.160	333.873	-3.71252	1.000	no_name
o14	330.160	333.873	-3.71252	1.000	no_name
o15	364.979	367.807	-2.82796	1.000	no_name
o16	418.913	421.595	-2.68214	1.000	no_name
o17	418.913	421.595	-2.68214	1.000	no_name
o18	418.913	421.595	-2.68214	1.000	no_name
o19	434.772	435.933	-1.16022	1.000	no_name
o20	477.439	476.538	0.900897	1.000	no_name
o21	485.543	483.266	2.27676	1.000	no_name
o22	486.385	483.923	2.46255	1.000	no_name
o23	490.075	486.583	3.49165	1.000	no_name
o24	490.075	486.583	3.49165	1.000	no_name

See file PEST_PESTICIDE.RES for more details of residuals in graph-ready format.

See file PEST_PESTICIDE.SEO for composite observation sensitivities.

Objective function ----->

Sum of squared weighted residuals (ie phi) = 296.8

Correlation Coefficient ----->

Correlation coefficient = 0.9999

Analysis of residuals ----->

All residuals:-

Number of residuals with non-zero weight	= 24
Mean value of non-zero weighted residuals	= 0.6786
Maximum weighted residual [observation "o10"]	= 11.01
Minimum weighted residual [observation "o13"]	= -3.713
Standard variance of weighted residuals	= 13.49
Standard error of weighted residuals	= 3.673

Note: the above variance was obtained by dividing the objective function by the number of system degrees of freedom (ie. number of observations with non-zero weight plus number of prior information articles with non-zero weight minus the number of adjustable parameters.) If the degrees of freedom is negative the divisor becomes the number of observations with non-zero weight plus the number of prior information items with non-zero weight.

Parameter covariance matrix ----->

	koc	kdeg
koc	5.5159E-03	3.6736E-07
kdeg	3.6736E-07	7.1906E-10

Parameter correlation coefficient matrix ----->

	koc	kdeg
koc	1.000	0.1845
kdeg	0.1845	1.000

Normalized eigenvectors of parameter covariance matrix ----->

	Vector_1	Vector_2
koc	6.6602E-05	-1.000
kdeg	-1.000	-6.6602E-05

Eigenvalues ----->

6.9459E-10	5.5159E-03

Parameter	Estimated value	95% percent confidence limits lower limit	upper limit
koc	14.7900	14.6360	14.9440
DT50	20.98	20.94	21.01

Minimum error for which the Chi²-Test passes according to FOCUS: 1.23 %

8.1.2. Optimisation of pesticide fate

InversePELMO control file “sampling pesticide.txt”

```
01      05      01      0       24      2.5
31      5       1       0       1
30      6       1       0       1
31      7       1       0       1
31      8       1       0       1
30      9       1       0       1
31      10      1       0       1
30      11      1       0       1
31      12      1       1.46124 1
31      1       2       25.03332        1
28      2       2       112.65269       1
31      3       2       215.17544       1
30      4       2       273.90689       1
31      5       2       330.16014       1
30      6       2       330.16014       1
31      7       2       364.9787        1
31      8       2       418.91302       1
30      9       2       418.91302       1
31      10      2       418.91302       1
30      11      2       434.77234       1
31      12      2       477.43926       1
31      1       3       485.54307       1
28      2       3       486.38523       1
31      3       3       490.07456       1
30      4       3       490.07456       1
```

PEST control file “Pest_pesticide.pst”

```
 pcf
* control data
restart
   2  24   2  0
    1     1 single point
  5.0   2.0   0.3  0.03    10
  3.0   3.0 0.001
  0.1
   30  0.01     3     3  0.01     3
    1     1     1
* group definitions and derivative data
KOC  relative 0.01  0.0  switch  2.0 parabolic
KDEG  relative 0.01  0.0  switch  2.0 parabolic
* parameter data
KOC  none relative 5 1 1000 KOC       1.0000       0.00000
KDEG  none relative 1.09861228866811E-02 6.93147180559945E-04 0.693147180559945 KDEG
1.0000       0.00000
* observation data
o1    0                    1
o2    0                    1
o3    0                    1
o4    0                    1
o5    0                    1
o6    0                    1
o7    0                    1
o8    1.46124                    1
o9    25.03332                    1
o10    112.65269                    1
o11    215.17544                    1
o12    273.90689                    1
o13    330.16014                    1
o14    330.16014                    1
o15    364.9787                    1
o16    418.91302                    1
o17    418.91302                    1
o18    418.91302                    1
o19    434.77234                    1
o20    477.43926                    1
o21    485.54307                    1
o22    486.38523                    1
o23    490.07456                    1
o24    490.07456                    1
* model command line
run_pesticide
* model input/output
pesticide.tpl  Pesticide_B_example_1.psm
pest.ins pest_flux.plm
* prior information
```

PELMO output file “PEST_flux.plm”

```
0031 31 05 01  0
0061 30 06 01  0
0092 31 07 01  0
0123 31 08 01  0
0153 30 09 01  0
0184 31 10 01  0.0000019122
0214 30 11 01  0.00010610627
0245 31 12 01  0.51728890627
0276 31 01 02  17.42258290627
0304 28 02 02  101.64738290627
0335 31 03 02  210.59816290627
0365 30 04 02  274.92216290627
0396 31 05 02  333.87266290627
0426 30 06 02  333.87266290627
0457 31 07 02  367.80666290627
0488 31 08 02  421.59516290627
0518 30 09 02  421.59516290627
0549 31 10 02  421.59516290627
0579 30 11 02  435.93256290627
0610 31 12 02  476.53836290627
0641 31 01 03  483.26630590627
0669 28 02 03  483.92267590627
0700 31 03 03  486.58290790627
0730 30 04 03  486.58290790627
```

PEST output file “Pest_pesticide.rec”

```
                PEST RUN RECORD: CASE PEST_PESTICIDE


PEST run mode:-

   Parameter estimation mode


Case dimensions:-

   Number of parameters                :    2
   Number of adjustable parameters     :    2
   Number of parameter groups          :    2
   Number of observations              :   24
   Number of prior estimates           :    0


Model command line(s):-

   run_pesticide


Jacobian command line:-

   na


Model interface files:-

   Templates:
      PESTICIDE.TPL
   for model input files:
      PESTICIDE_B_EXAMPLE_1.PSM

   (Parameter values written using single precision protocol.)
   (Decimal point always included.)

   Instruction files:
      PEST.INS
   for reading model output files:
      PEST_FLUX.PLM


PEST-to-model message file:-

   na


Derivatives calculation:-

Param        Increment   Increment   Increment   Forward or   Multiplier  Method
group        type                    low bound   central      (central)   (central)
koc          relative    1.0000E-02   none        switch        2.000     parabolic
kdeg         relative    1.0000E-02   none        switch        2.000     parabolic


Parameter definitions:-

Name         Trans-            Change       Initial        Lower          Upper
             formation         limit        value          bound          bound
koc          none              relative    5.00000        1.00000        1000.00
kdeg         none              relative   1.099000E-02   6.900000E-04   0.693150

Name         Group          Scale         Offset        Model command number
koc          koc           1.00000        0.00000            1
kdeg         kdeg          1.00000        0.00000            1


Prior information:-

   No prior information supplied


Observations:-

Observation name    Observation       Weight       Group
```

```
 o1                  0.00000          1.000       no_name
 o2                  0.00000          1.000       no_name
 o3                  0.00000          1.000       no_name
 o4                  0.00000          1.000       no_name
 o5                  0.00000          1.000       no_name
 o6                  0.00000          1.000       no_name
 o7                  0.00000          1.000       no_name
 o8                  1.46124          1.000       no_name
 o9                  25.0333          1.000       no_name
 o10                 112.653          1.000       no_name
 o11                 215.175          1.000       no_name
 o12                 273.907          1.000       no_name
 o13                 330.160          1.000       no_name
 o14                 330.160          1.000       no_name
 o15                 364.979          1.000       no_name
 o16                 418.913          1.000       no_name
 o17                 418.913          1.000       no_name
 o18                 418.913          1.000       no_name
 o19                 434.772          1.000       no_name
 o20                 477.439          1.000       no_name
 o21                 485.543          1.000       no_name
 o22                 486.385          1.000       no_name
 o23                 490.075          1.000       no_name
 o24                 490.075          1.000       no_name


Control settings:-

   Initial lambda                                                :  5.0000
   Lambda adjustment factor                                      :  2.0000
   Sufficient new/old phi ratio per optimisation iteration       : 0.30000
   Limiting relative phi reduction between lambdas               : 3.00000E-02
   Maximum trial lambdas per iteration                           :  10

   Maximum  factor  parameter change (factor-limited changes)    :   na
   Maximum relative parameter change (relative-limited changes)  :  3.0000
   Fraction of initial parameter values used in computing
   change limit for near-zero parameters                         : 1.00000E-03
   Allow bending of parameter upgrade vector                     : no
   Allow parameters to stick to their bounds                     : no

   Relative phi reduction below which to begin use of
   central derivatives                                           : 0.10000

   Relative phi reduction indicating convergence                 : 0.10000E-01
   Number of phi values required within this range               :   3
   Maximum number of consecutive failures to lower phi           :   3
   Minimal relative parameter change indicating convergence      : 0.10000E-01
   Number of consecutive iterations with minimal param change    :   3
   Maximum number of optimisation iterations                     :  30

   Attempt automatic user intervention                           : no


                            OPTIMISATION RECORD


INITIAL CONDITIONS:
   Sum of squared weighted residuals (ie phi) =  6.10098E+05

      Current parameter values
      koc              5.00000
      kdeg            1.099000E-02


OPTIMISATION ITERATION NO.        :    1
   Model calls so far             :    1
   Starting phi for this iteration:  6.10098E+05

       Lambda =   5.0000     ----->
          Phi =  1.65784E+05  (  0.272 of starting phi)

   No more lambdas: phi is less than 0.3000 of starting phi
   Lowest phi this iteration:  1.65784E+05

      Current parameter values                Previous parameter values
      koc              5.00600                koc              5.00000
      kdeg            1.560000E-02            kdeg            1.099000E-02
   Maximum relative change: 0.4195     ["kdeg"]
```

```
OPTIMISATION ITERATION NO.        :    2
   Model calls so far             :    4
   Starting phi for this iteration:  1.65784E+05

       Lambda =   2.5000     ----->
          Phi =  1.56340E+05  (  0.943 of starting phi)

       Lambda =   1.2500     ----->
          Phi =  1.55900E+05  (  0.940 of starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:  1.55900E+05
   Relative phi reduction between optimisation iterations less than 0.1000
   Switch to central derivatives calculation

      Current parameter values                Previous parameter values
      koc              5.04200                koc              5.00600
      kdeg           1.671000E-02             kdeg           1.560000E-02
   Maximum relative change: 7.1154E-02 ["kdeg"]


OPTIMISATION ITERATION NO.        :    3
   Model calls so far             :    8
   Starting phi for this iteration:  1.55900E+05

       Lambda =  0.62500     ----->
          Phi =  9.59417E+05  (  6.154 times starting phi)

       Lambda =  0.31250     ----->
          Phi =  1.60826E+06  ( 10.316 times starting phi)

       Lambda =   1.2500     ----->
          Phi =  1.80902E+05  (  1.160 times starting phi)

       Lambda =   2.5000     ----->
          Phi =  1.33430E+05  (  0.856 of starting phi)

       Lambda =   5.0000     ----->
          Phi =  1.51729E+05  (  0.973 of starting phi)

   No more lambdas: phi rising
   Lowest phi this iteration:  1.33430E+05

      Current parameter values                Previous parameter values
      koc              6.01900                koc              5.04200
      kdeg           2.063000E-02             kdeg           1.671000E-02
   Maximum relative change: 0.2346     ["kdeg"]


OPTIMISATION ITERATION NO.        :    4
   Model calls so far             :   17
   Starting phi for this iteration:  1.33430E+05

       Lambda =   2.5000     ----->
          Phi =  1.31355E+05  (  0.984 of starting phi)

       Lambda =   1.2500     ----->
          Phi =  1.30446E+05  (  0.978 of starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:  1.30446E+05

      Current parameter values                Previous parameter values
      koc              6.10300                koc              6.01900
      kdeg           2.147000E-02             kdeg           2.063000E-02
   Maximum relative change: 4.0717E-02 ["kdeg"]


OPTIMISATION ITERATION NO.        :    5
   Model calls so far             :   23
   Starting phi for this iteration:  1.30446E+05

       Lambda =  0.62500     ----->
          Phi =  1.19313E+05  (  0.915 of starting phi)

       Lambda =  0.31250     ----->
          Phi =   91098.      (  0.698 of starting phi)

       Lambda =  0.15625     ----->
          Phi =  2.56993E+05  (  1.970 times starting phi)

   No more lambdas: phi rising
```

```
   Lowest phi this iteration:   91098.

      Current parameter values                Previous parameter values
      koc              7.81500                koc               6.10300
      kdeg           2.668000E-02             kdeg            2.147000E-02
   Maximum relative change: 0.2805     ["koc"]


OPTIMISATION ITERATION NO.        :    6
   Model calls so far             :   30
   Starting phi for this iteration:   91098.

       Lambda =  0.15625     ----->
          Phi =  1.92513E+05  (  2.113 times starting phi)

       Lambda =  7.81250E-02 ----->
          Phi =  4.90305E+05  (  5.382 times starting phi)

       Lambda =  0.31250     ----->
          Phi =   47871.      (  0.525 of starting phi)

       Lambda =  0.62500     ----->
          Phi =   72670.      (  0.798 of starting phi)

   No more lambdas: phi rising
   Lowest phi this iteration:   47871.

      Current parameter values                Previous parameter values
      koc              10.2400                koc               7.81500
      kdeg           3.122000E-02             kdeg            2.668000E-02
   Maximum relative change: 0.3103     ["koc"]


OPTIMISATION ITERATION NO.        :    7
   Model calls so far             :   38
   Starting phi for this iteration:   47871.

       Lambda =  0.31250     ----->
          Phi =   15984.      (  0.334 of starting phi)

       Lambda =  0.15625     ----->
          Phi =   19112.      (  0.399 of starting phi)

       Lambda =  0.62500     ----->
          Phi =   29252.      (  0.611 of starting phi)

   No more lambdas: phi rising
   Lowest phi this iteration:   15984.

      Current parameter values                Previous parameter values
      koc              12.1100                koc               10.2400
      kdeg           3.225000E-02             kdeg            3.122000E-02
   Maximum relative change: 0.1826     ["koc"]


OPTIMISATION ITERATION NO.        :    8
   Model calls so far             :   45
   Starting phi for this iteration:   15984.

       Lambda =  0.31250     ----->
          Phi =   11485.      (  0.719 of starting phi)

       Lambda =  0.15625     ----->
          Phi =   12288.      (  0.769 of starting phi)

       Lambda =  0.62500     ----->
          Phi =   9905.7      (  0.620 of starting phi)

       Lambda =   1.2500     ----->
          Phi =   6987.3      (  0.437 of starting phi)

       Lambda =   2.5000     ----->
          Phi =   2734.8      (  0.171 of starting phi)

   No more lambdas: phi is less than 0.3000 of starting phi
   Lowest phi this iteration:   2734.8

      Current parameter values                Previous parameter values
      koc              14.4200                koc               12.1100
      kdeg           3.334000E-02             kdeg            3.225000E-02
   Maximum relative change: 0.1908     ["koc"]
```

```
OPTIMISATION ITERATION NO.        :    9
   Model calls so far             :   54
   Starting phi for this iteration:   2734.8

       Lambda =   2.5000     ----->
          Phi =   478.67      (  0.175 of starting phi)

   No more lambdas: phi is less than 0.3000 of starting phi
   Lowest phi this iteration:   478.67

      Current parameter values                Previous parameter values
      koc              14.5200                koc               14.4200
      kdeg           3.300000E-02             kdeg            3.334000E-02
   Maximum relative change: 1.0198E-02 ["kdeg"]


OPTIMISATION ITERATION NO.        :   10
   Model calls so far             :   59
   Starting phi for this iteration:   478.67

       Lambda =   1.2500     ----->
          Phi =   309.72      (  0.647 of starting phi)

       Lambda =  0.62500     ----->
          Phi =   300.94      (  0.629 of starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:   300.94

      Current parameter values                Previous parameter values
      koc              14.7800                koc               14.5200
      kdeg           3.305000E-02             kdeg            3.300000E-02
   Maximum relative change: 1.7906E-02 ["koc"]


OPTIMISATION ITERATION NO.        :   11
   Model calls so far             :   65
   Starting phi for this iteration:   300.94

       Lambda =  0.31250     ----->
          Phi =   296.85      (  0.986 of starting phi)

       Lambda =  0.15625     ----->
          Phi =   296.85      (  0.986 of starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:   296.85

      Current parameter values                Previous parameter values
      koc              14.7900                koc               14.7800
      kdeg           3.304000E-02             kdeg            3.305000E-02
   Maximum relative change: 6.7659E-04 ["koc"]


OPTIMISATION ITERATION NO.        :   12
   Model calls so far             :   71
   Starting phi for this iteration:   296.85

       Lambda =  0.15625     ----->
          Phi =   296.85      (  1.000 times starting phi)

       Lambda =  7.81250E-02 ----->
          Phi =   296.85      (  1.000 times starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:   296.85

      Current parameter values                Previous parameter values
      koc              14.7900                koc               14.7900
      kdeg           3.304000E-02             kdeg            3.304000E-02
   Maximum relative change:  0.000     ["koc"]


OPTIMISATION ITERATION NO.        :   13
   Model calls so far             :   75
   Starting phi for this iteration:   296.85

       Lambda =  7.81250E-02 ----->
          Phi =   296.85      (  1.000 times starting phi)

       Lambda =  3.90625E-02 ----->
```

```
         Phi =   296.85      (  1.000 times starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:   296.85

      Current parameter values                Previous parameter values
      koc              14.7900                koc               14.7900
      kdeg           3.304000E-02             kdeg            3.304000E-02
   Maximum relative change:  0.000     ["koc"]

   Optimisation complete: relative parameter change less than 1.0000E-02
                          over  3 successive iterations.
   Total model calls:   79

   The model has been run one final time using best parameters.
   Thus all model input files contain best parameter values, and model
   output files contain model results based on these parameters.


                            OPTIMISATION RESULTS


Parameters ----->

Parameter        Estimated         95% percent confidence limits
                 value             lower limit       upper limit
 koc             14.7900            14.6360           14.9440
 kdeg          3.304000E-02       3.298439E-02      3.309561E-02

Note: confidence limits provide only an indication of parameter uncertainty.
      They rely on a linearity assumption which  may not extend as far in
      parameter space as the confidence limits themselves - see PEST manual.

See file PEST_PESTICIDE.SEN for parameter sensitivities.


Observations ----->

Observation      Measured       Calculated     Residual       Weight     Group
                 value          value
 o1              0.00000        0.00000        0.00000        1.000      no_name
 o2              0.00000        0.00000        0.00000        1.000      no_name
 o3              0.00000        0.00000        0.00000        1.000      no_name
 o4              0.00000        0.00000        0.00000        1.000      no_name
 o5              0.00000        0.00000        0.00000        1.000      no_name
 o6              0.00000       1.912200E-06  -1.912200E-06    1.000      no_name
 o7              0.00000       1.061063E-04  -1.061063E-04    1.000      no_name
 o8              1.46124       0.517289       0.943951        1.000      no_name
 o9              25.0333        17.4226        7.61074        1.000      no_name
 o10             112.653        101.647        11.0053        1.000      no_name
 o11             215.175        210.598        4.57728        1.000      no_name
 o12             273.907        274.922       -1.01527        1.000      no_name
 o13             330.160        333.873       -3.71252        1.000      no_name
 o14             330.160        333.873       -3.71252        1.000      no_name
 o15             364.979        367.807       -2.82796        1.000      no_name
 o16             418.913        421.595       -2.68214        1.000      no_name
 o17             418.913        421.595       -2.68214        1.000      no_name
 o18             418.913        421.595       -2.68214        1.000      no_name
 o19             434.772        435.933       -1.16022        1.000      no_name
 o20             477.439        476.538       0.900897        1.000      no_name
 o21             485.543        483.266        2.27676        1.000      no_name
 o22             486.385        483.923        2.46255        1.000      no_name
 o23             490.075        486.583        3.49165        1.000      no_name
 o24             490.075        486.583        3.49165        1.000      no_name

See file PEST_PESTICIDE.RES for more details of residuals in graph-ready format.

See file PEST_PESTICIDE.SEO for composite observation sensitivities.


Objective function ----->

  Sum of squared weighted residuals (ie phi)               =   296.8


Correlation Coefficient ----->

  Correlation coefficient                                  =  0.9999


Analysis of residuals ----->
```

All residuals:-

Number of residuals with non-zero weight	= 24
Mean value of non-zero weighted residuals	= 0.6786
Maximum weighted residual [observation "o10"]	= 11.01
Minimum weighted residual [observation "o13"]	= -3.713
Standard variance of weighted residuals	= 13.49
Standard error of weighted residuals	= 3.673

Note: the above variance was obtained by dividing the objective function by the number of system degrees of freedom (ie. number of observations with non-zero weight plus number of prior information articles with non-zero weight minus the number of adjustable parameters.) If the degrees of freedom is negative the divisor becomes the number of observations with non-zero weight plus the number of prior information items with non-zero weight.

Parameter covariance matrix ----->

	koc	kdeg
koc	5.5159E-03	3.6736E-07
kdeg	3.6736E-07	7.1906E-10

Parameter correlation coefficient matrix ----->

	koc	kdeg
koc	1.000	0.1845
kdeg	0.1845	1.000

Normalized eigenvectors of parameter covariance matrix ----->

	Vector_1	Vector_2
koc	6.6602E-05	-1.000
kdeg	-1.000	-6.6602E-05

Eigenvalues ----->

6.9459E-10 5.5159E-03

Parameter	Estimated value	95% percent confidence limits lower limit	upper limit
koc	14.7900	14.6360	14.9440
DT50	20.98	20.94	21.01

Minimum error for which the Chi²-Test passes according to FOCUS: 1.23 %

PELMO output file “ECHO.PLM”

```
1
 *********************************
 *                               *
 *   PESTICIDE LEACHING MODEL    *
 *   PELMO 4.00, Dec 2010        *
 *                               *
 *                               *
 *********************************


 DEVELOPED BY:
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  PELMO 4.00,       Dec 2010


***************HYDROLOGY DATAS**************

          YEAR  1: Hamburg 1978 (normal)
          YEAR  2: Hamburg 1961 (naá)
          YEAR  3: Hamburg 1978 (normal)



 HYDROLOGY AND SEDIMENT RELATED PARAMETERS
 ----------------------------------------

Temperature data are used to calculate pan evaporation.


  LATTITUDE OF THE LOCATION:  50.00

 PAN COEFFICIENT FOR EVAPORATION (NO CROP)           0.9805
 PAN COEFFICIENT FOR EVAPORATION (MID  SEASON)        1.340
 PAN COEFFICIENT FOR EVAPORATION (LATE SEASON)        4.072
 FLAG FOR ET (0=EVAP,1=TEMP,2=EVAP/TEMP,3=HAUDE)          1
 DEPTH TO WHICH ET IS COMPUTED YEAR-ROUND [CM]        30.00

 MONTHLY DAYLIGHT HOURS
    MONTH     DAY HOURS      MONTH     DAY HOURS      MONTH     DAY HOURS
    JAN.       8.312         FEB.       9.681         MAR.       11.64
    APR.       13.76         MAY        15.40         JUNE       16.12
    JULY       15.73         AUG.       14.31         SEP.       12.28
    OCT.       10.18         NOV.       8.561         DEC.       7.874

 SNOW MELT COEFFICIENT [CM/DEG-C-DAY]               0.4600
 INITIAL CROP NUMBER                                     3
 INITIAL CROP CONDITION                                  1



NO CALCULATION OF RUNOFF EVENTS
 CROP INFORMATION
 ----------------

        MAXIMUM                                    IRRIGATION PERENNIAL TILLAGE   SURFACE
        INTERCEPT.MAXIMUM     MAXIMUM   MAXIMUM      FLAG    CROP        FLAG    CONDITION
USLE COVER MANAGEMENT
 CROP   POTENTIAL ROOT DEPTH  COVER     WEIGHT       (0=NO)  (0=NO)    (0=NO)    AFTER
AMC         RUNOFF CURVE NUMBERS     "C" FACTOR
```

```
 NUMBER   [CM]      [CM]       [%]      [KG/M**2]   (1=YES)  (1=YES)   (1=YES)   HARVEST
FALLOW     CROP  RESIDUE   FALLOW  CROP    RESIDUE

I           72       67       72
    3     0.0000     100.0     90.00    0.0000        0          0         0         3
II          86       83       86   1.0000  1.0000  1.0000

III         94       92       94
```

CROP ROTATION INFORMATION

CROP NUMBER	TILLAGE DATE	EMERGENCE DATE	MATURATION DATE	SENESCENCE DATE	HARVEST DATE
Sillage Maize		5 MAY , 1	15 SEP., 1	21 AUG., 1	20 OCT., 1
Sillage Maize		5 MAY , 2	15 SEP., 2	21 AUG., 1	20 OCT., 2
Sillage Maize		5 MAY , 3	15 SEP., 3	21 AUG., 1	20 OCT., 3
Sillage Maize		5 MAY , 4	15 SEP., 4	21 AUG., 1	20 OCT., 4

*** PARAMETERS OF ACTIVE SUBSTANCE (FOCUS DUMMY B)***
****

PESTICIDE APPLICATION INFORMATION

APPLICATION DATE	PESTICIDE APPLIED [KG/HA]	INCORPORATION DEPTH [CM]
1 MAY , 1	1.000	0.0000

PLANT PESTICIDE PARAMETERS

MODEL UTILIZED (1=SOIL,2=LINEAR,3=EXPONENTIAL 1

VOLATILIZATION PARAMETERS ACTIVE SUBSTANCE

TEMPERATURE [deg C]	20.00
HENRY-CONSTANT [Pa*m3/mole] or [J/mole] CALCULATED USING	0.3333E-03
VAPOUR PRESSURE [Pa]	0.1000E-03
MOLECULAR MASS [g/mole]	300.0
WATER SOLUBILITY [mg/l]	90.00
TEMPERATURE [deg C]	30.00
HENRY-CONSTANT [Pa*m3/mole] or [J/mole] CALCULATED USING	0.3333E-03
VAPOUR PRESSURE [Pa]	0.1000E-03
MOLECULAR MASS [g/mole]	300.0
WATER SOLUBILITY [mg/l]	90.00
Q10-Factor for Henry's constant:	1.000
DIFFUSION COEFF.AIR [cm2/d]	4303.
DEPTH OF SURFACE LAYER FOR VOLATILIZATION [CM]	0.1000
HENRY CONSTANT AT 20.0 deg C [-]	0.1368E-06
HENRY CONSTANT AT 30.0 deg C [-]	0.1322E-06

PLANT UPTAKE OF ACTIVE SUBSTANCE

PLANT UPTAKE FACTOR (-)	0.5000

TRANSFORMATION PARAMETERS

TRANSFORM. TO	TRANSFORM. in EQ.Domaine	TEMP. OF STUDY	Q10 VALUE	MOISTURE-DURING-STUDY ABSOLUTE	MOISTURE RELATIVE	REL. EXPONENT	TRANSFORM IN NEQ DOMAIN

	[/DAY]	[C]	[-]	[%]	[%]	[-]	[-]
MET. A1	0.1000E-09	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
MET. B1	0.1000E-09	20.00	2.000	19.00	0.0000	0.0000	0.0000
MET. C1	0.1000E-09	20.00	2.000	19.00	0.0000	0.0000	0.0000
MET. D1	0.1000E-09	20.00	2.000	19.00	0.0000	0.0000	0.0000
BR/CO2	0.3304E-01	20.00	2.580	0.0000	100.0	0.7000	0.0000

SORPTION PARAMETERS

--PARAMETERS TO CALCULATE KD-VALUES WITH KOC--

KOC [CM**3/G]	14.79
FREUNDLICH-SORPTION EXPONENT 1/n	0.9000
[PEARL] FACTOR DESCRIBING NON-EQ-SITES EQ-SITES (-):	0.0000
[PEARL] DESORPTION RATE [1/D]:	0.0000
MIN. CONC FOR FREUNDLICH-SORPTION [æG/L]	0.1000E-19

DEPTH DEPENDEND SORPTION AND TRANSFORMATION PARAMETERS

HORIZON	KOC	KD	FR-EXP	TRANSFORMATION RATE TO MET. A1	MET. B1	MET. C1	MET. D1	BR/CO2
	[CM**3/G]	[CM**3/G]	[-]	[/DAY]	[/DAY]	[/DAY]	[/DAY]	[/DAY]
1	14.79	0.2219	0.9000	0.1000E-09	0.1000E-09	0.1000E-09	0.1000E-09	0.3304E-01
2	14.79	0.1479	0.9000	0.1600E-10	0.1600E-10	0.1600E-10	0.1600E-10	0.5286E-02
3	14.79	0.2958E-01	0.9000	0.9000E-11	0.9000E-11	0.9000E-11	0.9000E-11	0.2974E-02
4	0.0000	0.0000	0.9000	0.1300E-10	0.1300E-10	0.1300E-10	0.1300E-10	0.4295E-02
5	0.0000	0.0000	0.9000	0.0000	0.0000	0.0000	0.0000	0.0000

Pest
Borstel Mais Mais Mais

GENERAL SOIL INFORMATION

CORE DEPTH [CM]		110.0
TOTAL HORIZONS IN CORE		5
TOTAL COMPARTMENTS IN CORE		44
DPFLAG FLAG	(0=DISP.COEFF.1=DISP.LENGTH)	0
THETA FLAG	(0=INPUT,1=PRZM 2=PELMO)	2
PARTITION COEFFICIENT FLAG	(0=INPUT,1=CALCULATED)	1
BULK DENSITY FLAG	(0=INPUT,1=CALCULATED)	0
SOIL HYDRAULICS MODULE		free drainage

SOIL HORIZON INFORMATION

HORIZON	THICKNESS [CM]	BULK DENSITY [G/CM**3]	INITIAL SOIL WATER CONTENT [CM/CM]	DRAINAGE PARAMETER [/DAY]	SAND [%]	CLAY [%]	ORGANIC CARBON [%]	DISPERSION COEFFICIENT [CM**2/DAY]	BIODEG. FACTOR [-]	PH [-]
1	30.0000	1.5000	0.2000	2.3000	68.3000	7.2000	1.5000	0.0000	1.0000	5.7000
2	30.0000	1.6000	0.2000	2.3000	67.0000	6.7000	1.0000	0.0000	0.1600	4.9000
3	15.0000	1.5800	0.2000	2.2000	96.2000	0.9000	0.2000	0.0000	0.0900	4.9000
4	15.0000	1.6200	0.2000	0.0000	99.8000	0.0000	0.0000	0.0000	0.1300	5.0000
5	20.0000	1.6000	0.2000	0.0000	100.0000	0.0000	0.0000	0.0000	0.0000	4.8000

OUTPUT FILE PARAMETERS

OUTPUT	TIME STEP	LAYER FREQ
WATR	DAY	1
PEST	DAY	1

CONC DAY 1

CALCULATED HYDRAULIC PROPERTIES

HORIZON	FIELD CAPACITY [CM3/CM3]	WILTING POINT [CM3/CM3]
1	0.2778	0.0592
2	0.2794	0.0586
3	0.2094	0.0336
4	0.2004	0.0301
5	0.2000	0.0300

Total number of layers in the top meter: 41

PLOT FILE INFORMATION

NUMBER OF PLOTTING VARIABLES 1

TIMSER NAME	MODE	DEPTH(CM)	ARGUMENT	CONSTANT	SUBSTANCE
LEAC	TSER	100.	41	0.1000E+10	PESTIC

8.2. Example data set 2

8.2.1. Optimisation of soil hydrology

InversePELMO control file “sampling water.txt”

```
01      08      01
 10
31      8       1       47.9    1
31      10      1       124.6   1
30      11      1       177.35  1
31      12      1       222.4   1
31      1       2       255.5   1
28      2       2       346.9   1
31      8       2       495.25  1
31      10      2       582.9   1
30      11      2       675.9   1
31      12      2       767.15  1
```

PEST control file “Pest_water.pst”

```
pcf
* control data
restart
   4  10   4  0
    1     1 single point
  5.0   2.0   0.3  0.03    10
  3.0   3.0 0.001
  0.1
   30  0.01     3     3  0.01     3
    1     1     1
* group definitions and derivative data
Kc0  relative 0.01  0.0  switch  2.0 parabolic
Kc1  relative 0.01  0.0  switch  2.0 parabolic
Kc2  relative 0.01  0.0  switch  2.0 parabolic
MOI0  relative 0.01  0.0  switch  2.0 parabolic
* parameter data
Kc0  none relative 1 0.5 10 Kc0       1.0000       0.00000
Kc1  none relative 1 0.5 10 Kc1       1.0000       0.00000
Kc2  none relative 1 0.5 10 Kc2       1.0000       0.00000
MOI0    none relative 0.2 0.05 0.5 MOI0       1.0000       0.00000
* observation data
o1    47.9                    1
o2    124.6                    1
o3    177.35                    1
o4    222.4                    1
o5    255.5                    1
o6    346.9                    1
o7    495.25                    1
o8    582.9                    1
o9    675.9                    1
o10    767.15                    1
* model command line
run_water
* model input/output
scenario.tpl  BORSTEL.SZE
pest.ins pest_water.plm
* prior information
```

PELMO output file “PEST_water.plm”

```
0031 31 08 01  69.143
0092 31 10 01  120.7133
0122 30 11 01  171.0434
0153 31 12 01  221.62815
0184 31 01 02  264.20235
0212 28 02 02  331.35835
0396 31 08 02  451.87768
0457 31 10 02  564.81468
0487 30 11 02  710.48953
0518 31 12 02  790.618272
```

PEST output file “Pest_water.rec”

```
                  PEST RUN RECORD: CASE PEST_WATER


PEST run mode:-

   Parameter estimation mode


Case dimensions:-

   Number of parameters                :    4
   Number of adjustable parameters     :    4
   Number of parameter groups          :    4
   Number of observations              :   10
   Number of prior estimates           :    0


Model command line(s):-

   run_water


Jacobian command line:-

   na


Model interface files:-

   Templates:
      SCENARIO.TPL
   for model input files:
      BORSTEL.SZE

   (Parameter values written using single precision protocol.)
   (Decimal point always included.)

   Instruction files:
      PEST.INS
   for reading model output files:
      PEST_WATER.PLM


PEST-to-model message file:-

   na


Derivatives calculation:-

Param        Increment   Increment   Increment   Forward or   Multiplier  Method
group        type                    low bound   central      (central)   (central)
kc0          relative    1.0000E-02   none        switch        2.000     parabolic
kc1          relative    1.0000E-02   none        switch        2.000     parabolic
kc2          relative    1.0000E-02   none        switch        2.000     parabolic
moi0         relative    1.0000E-02   none        switch        2.000     parabolic


Parameter definitions:-

Name         Trans-            Change       Initial        Lower          Upper
             formation         limit        value          bound          bound
kc0          none              relative    1.00000       0.500000        10.0000
kc1          none              relative    1.00000       0.500000        10.0000
kc2          none              relative    1.00000       0.500000        10.0000
moi0         none              relative   0.200000       5.000000E-02   0.500000

Name         Group          Scale         Offset        Model command number
kc0          kc0           1.00000        0.00000            1
kc1          kc1           1.00000        0.00000            1
kc2          kc2           1.00000        0.00000            1
moi0         moi0          1.00000        0.00000            1
```

Prior information:-

No prior information supplied

Observations:-

Observation name	Observation	Weight	Group
o1	47.9000	1.000	no_name
o2	124.600	1.000	no_name
o3	177.350	1.000	no_name
o4	222.400	1.000	no_name
o5	255.500	1.000	no_name
o6	346.900	1.000	no_name
o7	495.250	1.000	no_name
o8	582.900	1.000	no_name
o9	675.900	1.000	no_name
o10	767.150	1.000	no_name

Control settings:-

```
   Initial lambda                                                 :  5.0000
   Lambda adjustment factor                                       :  2.0000
   Sufficient new/old phi ratio per optimisation iteration        : 0.30000
   Limiting relative phi reduction between lambdas                : 3.00000E-02
   Maximum trial lambdas per iteration                            :  10

   Maximum  factor  parameter change (factor-limited changes)     :   na
   Maximum relative parameter change (relative-limited changes)   :  3.0000
   Fraction of initial parameter values used in computing
   change limit for near-zero parameters                          : 1.00000E-03
   Allow bending of parameter upgrade vector                      : no
   Allow parameters to stick to their bounds                      : no

   Relative phi reduction below which to begin use of
   central derivatives                                            : 0.10000

   Relative phi reduction indicating convergence                  : 0.10000E-01
   Number of phi values required within this range                :   3
   Maximum number of consecutive failures to lower phi            :   3
   Minimal relative parameter change indicating convergence       : 0.10000E-01
   Number of consecutive iterations with minimal param change     :   3
   Maximum number of optimisation iterations                      :  30

   Attempt automatic user intervention                            : no
```

OPTIMISATION RECORD

```
INITIAL CONDITIONS:
   Sum of squared weighted residuals (ie phi) =   56927.

      Current parameter values
      kc0              1.00000
      kc1              1.00000
      kc2              1.00000
      moi0            0.200000


OPTIMISATION ITERATION NO.        :    1
   Model calls so far             :    1
   Starting phi for this iteration:   56927.

   Parameter "kc0" has no effect on observations.
   Parameter "kc1" has no effect on observations.
   Parameter "kc2" has no effect on observations.

       Lambda =   5.0000     ----->
          Phi =   4984.2      (  0.088 of starting phi)

   No more lambdas: phi is less than 0.3000 of starting phi
   Lowest phi this iteration:   4984.2

      Current parameter values                Previous parameter values
      kc0              1.00000                kc0              1.00000
      kc1              1.00000                kc1              1.00000
      kc2              1.00000                kc2              1.00000
      moi0            0.285800                moi0            0.200000
   Maximum relative change: 0.4290     ["moi0"]
```

```
OPTIMISATION ITERATION NO.        :    2
   Model calls so far             :    6
   Starting phi for this iteration:   4984.2

   Parameter "kc0" has no effect on observations.
   Parameter "kc1" has no effect on observations.
   Parameter "kc2" has no effect on observations.

       Lambda =   2.5000     ----->
          Phi =   4779.6      (  0.959 of starting phi)

       Lambda =   1.2500     ----->
          Phi =   4779.6      (  0.959 of starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:   4779.6
   Relative phi reduction between optimisation iterations less than 0.1000
   Switch to central derivatives calculation

      Current parameter values                Previous parameter values
      kc0              1.00000                kc0              1.00000
      kc1              1.00000                kc1              1.00000
      kc2              1.00000                kc2              1.00000
      moi0            0.281140                moi0            0.285800
   Maximum relative change: 1.6305E-02 ["moi0"]


OPTIMISATION ITERATION NO.        :    3
   Model calls so far             :   12
   Starting phi for this iteration:   4779.6

   Parameter "kc0" has no effect on observations.
   Parameter "kc1" has no effect on observations.
   Parameter "kc2" has no effect on observations.

       Lambda =   1.2500     ----->
          Phi =   4779.4      (  1.000 of starting phi)

       Lambda =  0.62500     ----->
          Phi =   4779.4      (  1.000 of starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:   4779.4

      Current parameter values                Previous parameter values
      kc0              1.00000                kc0              1.00000
      kc1              1.00000                kc1              1.00000
      kc2              1.00000                kc2              1.00000
      moi0            0.280990                moi0            0.281140
   Maximum relative change: 5.3354E-04 ["moi0"]


OPTIMISATION ITERATION NO.        :    4
   Model calls so far             :   22
   Starting phi for this iteration:   4779.4

   Parameter "kc0" has no effect on observations.
   Parameter "kc1" has no effect on observations.
   Parameter "kc2" has no effect on observations.

       Lambda =  0.62500     ----->
          Phi =   4779.4      (  1.000 of starting phi)

       Lambda =  0.31250     ----->
          Phi =   4779.4      (  1.000 of starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:   4779.4

      Current parameter values                Previous parameter values
      kc0              1.00000                kc0              1.00000
      kc1              1.00000                kc1              1.00000
      kc2              1.00000                kc2              1.00000
      moi0            0.281000                moi0            0.280990
   Maximum relative change: 3.5588E-05 ["moi0"]

   Optimisation complete: the  3 lowest phi's are within a relative distance
                          of eachother of 1.000E-02
   Total model calls:   32
```

The model has been run one final time using best parameters.
Thus all model input files contain best parameter values, and model
output files contain model results based on these parameters.

OPTIMISATION RESULTS

Covariance matrix and parameter confidence intervals cannot be determined:-
Normal matrix nearly singular; cannot be inverted.

Parameters ----->

Parameter	Estimated value
kc0	1.00000
kc1	1.00000
kc2	1.00000
moi0	0.281000

See file PEST_WATER.SEN for parameter sensitivities.

Observations ----->

Observation	Measured value	Calculated value	Residual	Weight	Group
o1	47.9000	69.1430	-21.2430	1.000	no_name
o2	124.600	120.713	3.88670	1.000	no_name
o3	177.350	171.043	6.30660	1.000	no_name
o4	222.400	221.628	0.771850	1.000	no_name
o5	255.500	264.202	-8.70235	1.000	no_name
o6	346.900	331.358	15.5417	1.000	no_name
o7	495.250	451.878	43.3723	1.000	no_name
o8	582.900	564.815	18.0853	1.000	no_name
o9	675.900	710.490	-34.5895	1.000	no_name
o10	767.150	790.618	-23.4683	1.000	no_name

See file PEST_WATER.RES for more details of residuals in graph-ready format.

See file PEST_WATER.SEO for composite observation sensitivities.

Objective function ----->

Sum of squared weighted residuals (ie phi) = 4779.

Correlation Coefficient ----->

Correlation coefficient = 0.9958

Analysis of residuals ----->

All residuals:-
Number of residuals with non-zero weight = 10
Mean value of non-zero weighted residuals = -3.8712E-03
Maximum weighted residual [observation "o7"] = 43.37
Minimum weighted residual [observation "o9"] = -34.59
Standard variance of weighted residuals = 796.6
Standard error of weighted residuals = 28.22

Note: the above variance was obtained by dividing the objective
function by the number of system degrees of freedom (ie. number of
observations with non-zero weight plus number of prior information
articles with non-zero weight minus the number of adjustable parameters.)
If the degrees of freedom is negative the divisor becomes
the number of observations with non-zero weight plus the number of
prior information items with non-zero weight.

Covariance and other statistical matricies cannot be determined:-
Normal matrix nearly singular; cannot be inverted.

Minimum error for which the Chi²-Test passes according to FOCUS: 4.75 %

8.2.2. Optimisation of pesticide fate

InversePELMO control file “sampling pesticide.txt”

```
01      08      01      0       10      5
31      8       1       0       1
31      10      1       0       1
30      11      1       0       1
31      12      1       0       1
31      1       2       0       1
28      2       2       0       1
31      8       2       0       1
31      10      2       12.271  1
30      11      2       54.121  1
31      12      2       104.3085        1
```

PEST control file “Pest_pesticide.pst”

```
pcf
* control data
restart
   2  10   2  0
    1     1 single point
  5.0   2.0   0.3  0.03    10
  3.0   3.0 0.001
  0.1
   30  0.01     3     3  0.01     3
    1     1     1
* group definitions and derivative data
KOC  relative 0.01  0.0  switch  2.0 parabolic
KDEG  relative 0.01  0.0  switch  2.0 parabolic
* parameter data
KOC  none relative 50 1 1000 KOC       1.0000       0.00000
KDEG  none relative 1.09861228866811E-02 6.93147180559945E-04 0.693147180559945 KDEG
1.0000       0.00000
* observation data
o1    0                    1
o2    0                    1
o3    0                    1
o4    0                    1
o5    0                    1
o6    0                    1
o7    0                    1
o8    12.271                    1
o9    54.121                    1
o10    104.3085                    1
* model command line
run_pesticide
* model input/output
pesticide.tpl  Substance_2.psm
pest.ins pest_flux.plm
* prior information
```

PELMO output file “PEST_flux.plm”

```
0031 31 08 01  0
0092 31 10 01  5.4360315E-16
0122 30 11 01  7.517069544315E-11
0153 31 12 01  1.25404336295443E-07
0184 31 01 02  1.03420123362954E-05
0212 28 02 02  2.8029550123363E-03
0396 31 08 02  0.742968255012336
0457 31 10 02  9.71547825501234
0487 30 11 02  55.7414252550123
0518 31 12 02  103.614612255012
```

PEST output file “Pest_pesticide.rec”

```
                PEST RUN RECORD: CASE PEST_PESTICIDE


PEST run mode:-

   Parameter estimation mode


Case dimensions:-

   Number of parameters                :    2
   Number of adjustable parameters     :    2
   Number of parameter groups          :    2
   Number of observations              :   10
   Number of prior estimates           :    0


Model command line(s):-

   run_pesticide


Jacobian command line:-

   na


Model interface files:-

   Templates:
      PESTICIDE.TPL
   for model input files:
      SUBSTANCE_2.PSM

   (Parameter values written using single precision protocol.)
   (Decimal point always included.)

   Instruction files:
      PEST.INS
   for reading model output files:
      PEST_FLUX.PLM


PEST-to-model message file:-

   na


Derivatives calculation:-

Param        Increment   Increment   Increment   Forward or   Multiplier  Method
group        type                    low bound   central      (central)   (central)
koc          relative    1.0000E-02   none        switch        2.000     parabolic
kdeg         relative    1.0000E-02   none        switch        2.000     parabolic


Parameter definitions:-

Name         Trans-            Change       Initial        Lower          Upper
             formation         limit        value          bound          bound
koc          none              relative    50.0000        1.00000        1000.00
kdeg         none              relative   1.099000E-02   6.900000E-04   0.693150

Name         Group          Scale         Offset        Model command number
koc          koc           1.00000        0.00000            1
kdeg         kdeg          1.00000        0.00000            1


Prior information:-

   No prior information supplied


Observations:-

Observation name    Observation       Weight       Group
```

```
 o1                  0.00000          1.000       no_name
 o2                  0.00000          1.000       no_name
 o3                  0.00000          1.000       no_name
 o4                  0.00000          1.000       no_name
 o5                  0.00000          1.000       no_name
 o6                  0.00000          1.000       no_name
 o7                  0.00000          1.000       no_name
 o8                  12.2710          1.000       no_name
 o9                  54.1210          1.000       no_name
 o10                 104.309          1.000       no_name


Control settings:-

   Initial lambda                                                 :  5.0000
   Lambda adjustment factor                                       :  2.0000
   Sufficient new/old phi ratio per optimisation iteration        : 0.30000
   Limiting relative phi reduction between lambdas                : 3.00000E-02
   Maximum trial lambdas per iteration                            :  10

   Maximum  factor  parameter change (factor-limited changes)     :   na
   Maximum relative parameter change (relative-limited changes)   :  3.0000
   Fraction of initial parameter values used in computing
   change limit for near-zero parameters                          : 1.00000E-03
   Allow bending of parameter upgrade vector                      : no
   Allow parameters to stick to their bounds                      : no

   Relative phi reduction below which to begin use of
   central derivatives                                            : 0.10000

   Relative phi reduction indicating convergence                  : 0.10000E-01
   Number of phi values required within this range                :   3
   Maximum number of consecutive failures to lower phi            :   3
   Minimal relative parameter change indicating convergence       : 0.10000E-01
   Number of consecutive iterations with minimal param change     :   3
   Maximum number of optimisation iterations                      :  30

   Attempt automatic user intervention                            : no


                           OPTIMISATION RECORD


INITIAL CONDITIONS:
   Sum of squared weighted residuals (ie phi) =  6.20080E+08

      Current parameter values
      koc              50.0000
      kdeg            1.099000E-02


OPTIMISATION ITERATION NO.        :    1
   Model calls so far             :    1
   Starting phi for this iteration:  6.20080E+08

       Lambda =   5.0000     ----->
          Phi =  8.43319E+07  (  0.136 of starting phi)

   No more lambdas: phi is less than 0.3000 of starting phi
   Lowest phi this iteration:  8.43319E+07

      Current parameter values                Previous parameter values
      koc              50.0400                koc              50.0000
      kdeg            2.103000E-02            kdeg            1.099000E-02
   Maximum relative change: 0.9136     ["kdeg"]


OPTIMISATION ITERATION NO.        :    2
   Model calls so far             :    4
   Starting phi for this iteration:  8.43319E+07

       Lambda =   2.5000     ----->
          Phi =  1.14493E+07  (  0.136 of starting phi)

   No more lambdas: phi is less than 0.3000 of starting phi
   Lowest phi this iteration:  1.14493E+07

      Current parameter values                Previous parameter values
      koc              50.1100                koc              50.0400
      kdeg            3.124000E-02            kdeg            2.103000E-02
   Maximum relative change: 0.4855     ["kdeg"]
```

```
OPTIMISATION ITERATION NO.        :    3
   Model calls so far             :    7
   Starting phi for this iteration:  1.14493E+07

       Lambda =   1.2500     ----->
          Phi =  1.49660E+06  (  0.131 of starting phi)

   No more lambdas: phi is less than 0.3000 of starting phi
   Lowest phi this iteration:  1.49660E+06

      Current parameter values                Previous parameter values
      koc              50.2400                koc              50.1100
      kdeg            4.157000E-02            kdeg            3.124000E-02
   Maximum relative change: 0.3307     ["kdeg"]


OPTIMISATION ITERATION NO.        :    4
   Model calls so far             :   10
   Starting phi for this iteration:  1.49660E+06

       Lambda =  0.62500     ----->
          Phi =  1.81613E+05  (  0.121 of starting phi)

   No more lambdas: phi is less than 0.3000 of starting phi
   Lowest phi this iteration:  1.81613E+05

      Current parameter values                Previous parameter values
      koc              50.5300                koc              50.2400
      kdeg            5.155000E-02            kdeg            4.157000E-02
   Maximum relative change: 0.2401     ["kdeg"]


OPTIMISATION ITERATION NO.        :    5
   Model calls so far             :   13
   Starting phi for this iteration:  1.81613E+05

       Lambda =  0.31250     ----->
          Phi =   19869.      (  0.109 of starting phi)

   No more lambdas: phi is less than 0.3000 of starting phi
   Lowest phi this iteration:   19869.

      Current parameter values                Previous parameter values
      koc              51.2500                koc              50.5300
      kdeg            5.993000E-02            kdeg            5.155000E-02
   Maximum relative change: 0.1626     ["kdeg"]


OPTIMISATION ITERATION NO.        :    6
   Model calls so far             :   16
   Starting phi for this iteration:   19869.

       Lambda =  0.15625     ----->
          Phi =   3407.5      (  0.172 of starting phi)

   No more lambdas: phi is less than 0.3000 of starting phi
   Lowest phi this iteration:   3407.5

      Current parameter values                Previous parameter values
      koc              53.3100                koc              51.2500
      kdeg            6.387000E-02            kdeg            5.993000E-02
   Maximum relative change: 6.5743E-02 ["kdeg"]


OPTIMISATION ITERATION NO.        :    7
   Model calls so far             :   19
   Starting phi for this iteration:   3407.5

       Lambda =  7.81250E-02 ----->
          Phi =   1394.7      (  0.409 of starting phi)

       Lambda =  3.90625E-02 ----->
          Phi =   1095.6      (  0.322 of starting phi)

       Lambda =  1.95313E-02 ----->
          Phi =   2830.2      (  0.831 of starting phi)

   No more lambdas: phi rising
   Lowest phi this iteration:   1095.6
```

```
      Current parameter values                Previous parameter values
      koc              66.4100                koc               53.3100
      kdeg           5.008000E-02             kdeg            6.387000E-02
   Maximum relative change: 0.2457     ["koc"]


OPTIMISATION ITERATION NO.        :    8
   Model calls so far             :   24
   Starting phi for this iteration:   1095.6

       Lambda =  1.95313E-02 ----->
          Phi =   225.40      (  0.206 of starting phi)

   No more lambdas: phi is less than 0.3000 of starting phi
   Lowest phi this iteration:   225.40

      Current parameter values                Previous parameter values
      koc              78.1200                koc               66.4100
      kdeg           4.159000E-02             kdeg            5.008000E-02
   Maximum relative change: 0.1763     ["koc"]


OPTIMISATION ITERATION NO.        :    9
   Model calls so far             :   27
   Starting phi for this iteration:   225.40

       Lambda =  9.76563E-03 ----->
          Phi =   36.266      (  0.161 of starting phi)

   No more lambdas: phi is less than 0.3000 of starting phi
   Lowest phi this iteration:   36.266

      Current parameter values                Previous parameter values
      koc              89.3100                koc               78.1200
      kdeg           3.423000E-02             kdeg            4.159000E-02
   Maximum relative change: 0.1770     ["kdeg"]


OPTIMISATION ITERATION NO.        :   10
   Model calls so far             :   30
   Starting phi for this iteration:   36.266

       Lambda =  4.88281E-03 ----->
          Phi =   12.915      (  0.356 of starting phi)

       Lambda =  2.44141E-03 ----->
          Phi =   11.162      (  0.308 of starting phi)

       Lambda =  1.22070E-03 ----->
          Phi =   10.545      (  0.291 of starting phi)

   No more lambdas: phi is less than 0.3000 of starting phi
   Lowest phi this iteration:   10.545

      Current parameter values                Previous parameter values
      koc              94.2900                koc               89.3100
      kdeg           3.138000E-02             kdeg            3.423000E-02
   Maximum relative change: 8.3260E-02 ["kdeg"]


OPTIMISATION ITERATION NO.        :   11
   Model calls so far             :   35
   Starting phi for this iteration:   10.545

       Lambda =  6.10352E-04 ----->
          Phi =   10.203      (  0.968 of starting phi)

       Lambda =  3.05176E-04 ----->
          Phi =   10.203      (  0.968 of starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:   10.203
   Relative phi reduction between optimisation iterations less than 0.1000
   Switch to central derivatives calculation

      Current parameter values                Previous parameter values
      koc              95.1900                koc               94.2900
      kdeg           3.085000E-02             kdeg            3.138000E-02
   Maximum relative change: 1.6890E-02 ["kdeg"]


OPTIMISATION ITERATION NO.        :   12
```

```
   Model calls so far             :   39
   Starting phi for this iteration:   10.203

       Lambda =  3.05176E-04 ----->
          Phi =   10.190      (  0.999 of starting phi)

       Lambda =  1.52588E-04 ----->
          Phi =   10.190      (  0.999 of starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:   10.190

      Current parameter values                Previous parameter values
      koc              95.1700                koc              95.1900
      kdeg            3.086000E-02            kdeg            3.085000E-02
   Maximum relative change: 3.2415E-04 ["kdeg"]


OPTIMISATION ITERATION NO.        :   13
   Model calls so far             :   45
   Starting phi for this iteration:   10.190

       Lambda =  1.52588E-04 ----->
          Phi =   10.195      (  1.000 times starting phi)

       Lambda =  7.62939E-05 ----->
          Phi =   10.195      (  1.000 times starting phi)

   No more lambdas: relative phi reduction between lambdas less than 0.0300
   Lowest phi this iteration:   10.195

      Current parameter values                Previous parameter values
      koc              95.1600                koc              95.1700
      kdeg            3.086000E-02            kdeg            3.086000E-02
   Maximum relative change: 1.0508E-04 ["koc"]

   Optimisation complete: the  3 lowest phi's are within a relative distance
                          of eachother of 1.000E-02
   Total model calls:   51

   The model has been run one final time using best parameters.
   Thus all model input files contain best parameter values, and model
   output files contain model results based on these parameters.


                           OPTIMISATION RESULTS


Parameters ----->

Parameter        Estimated         95% percent confidence limits
                 value             lower limit       upper limit
 koc             95.1700            91.3826           98.9574
 kdeg           3.086000E-02       2.860899E-02      3.311101E-02

Note: confidence limits provide only an indication of parameter uncertainty.
      They rely on a linearity assumption which  may not extend as far in
      parameter space as the confidence limits themselves - see PEST manual.

See file PEST_PESTICIDE.SEN for parameter sensitivities.


Observations ----->

Observation      Measured       Calculated     Residual       Weight     Group
                 value          value
 o1              0.00000         0.00000         0.00000        1.000      no_name
 o2              0.00000        5.436032E-16  -5.436032E-16    1.000      no_name
 o3              0.00000        7.517070E-11  -7.517070E-11    1.000      no_name
 o4              0.00000        1.254043E-07  -1.254043E-07    1.000      no_name
 o5              0.00000        1.034201E-05  -1.034201E-05    1.000      no_name
 o6              0.00000        2.802955E-03  -2.802955E-03    1.000      no_name
 o7              0.00000        0.742968      -0.742968        1.000      no_name
 o8              12.2710         9.71548        2.55552        1.000      no_name
 o9              54.1210         55.7414       -1.62043        1.000      no_name
 o10             104.309         103.615        0.693888       1.000      no_name

See file PEST_PESTICIDE.RES for more details of residuals in graph-ready format.

See file PEST_PESTICIDE.SEO for composite observation sensitivities.
```

Objective function ----->

Sum of squared weighted residuals (ie phi) = 10.19

Correlation Coefficient ----->

Correlation coefficient = 0.9995

Analysis of residuals ----->

All residuals:-

Number of residuals with non-zero weight	= 10
Mean value of non-zero weighted residuals	= 8.8320E-02
Maximum weighted residual [observation "o8"]	= 2.556
Minimum weighted residual [observation "o9"]	= -1.620
Standard variance of weighted residuals	= 1.274
Standard error of weighted residuals	= 1.129

Note: the above variance was obtained by dividing the objective function by the number of system degrees of freedom (ie. number of observations with non-zero weight plus number of prior information articles with non-zero weight minus the number of adjustable parameters.) If the degrees of freedom is negative the divisor becomes the number of observations with non-zero weight plus the number of prior information items with non-zero weight.

Parameter covariance matrix ----->

	koc	kdeg
koc	2.698	-1.5992E-03
kdeg	-1.5992E-03	9.5288E-07

Parameter correlation coefficient matrix ----->

	koc	kdeg
koc	1.000	-0.9975
kdeg	-0.9975	1.000

Normalized eigenvectors of parameter covariance matrix ----->

	Vector_1	Vector_2
koc	-5.9283E-04	-1.000
kdeg	-1.000	5.9283E-04

Eigenvalues ----->

4.8263E-09 2.698

Parameter	Estimated value	95% percent confidence limits lower limit	upper limit
koc	95.1700	91.3826	98.9574
DT50	22.46	20.93	24.23

Minimum error for which the Chi²-Test passes according to FOCUS: 4.75 %

PELMO output file “ECHO.PLM”

```
1
 *********************************
 *                               *
 *   PESTICIDE LEACHING MODEL    *
 *   PELMO 4.00, Dec 2010        *
 *                               *
 *                               *
 *********************************


 DEVELOPED BY:
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  PELMO 4.00,       Dec 2010


***************HYDROLOGY DATAS**************

          YEAR  1: Grafschaft 1
          YEAR  2: Grafschaft 2


 HYDROLOGY AND SEDIMENT RELATED PARAMETERS
 ----------------------------------------

Temperature data are used to calculate pan evaporation.


  LATTITUDE OF THE LOCATION:  53.50

 PAN COEFFICIENT FOR EVAPORATION (NO CROP)            1.000
 PAN COEFFICIENT FOR EVAPORATION (MID  SEASON)        1.000
 PAN COEFFICIENT FOR EVAPORATION (LATE SEASON)        1.000
 FLAG FOR ET (0=EVAP,1=TEMP,2=EVAP/TEMP,3=HAUDE)          1
 DEPTH TO WHICH ET IS COMPUTED YEAR-ROUND [CM]        15.00

 MONTHLY DAYLIGHT HOURS
    MONTH     DAY HOURS      MONTH     DAY HOURS      MONTH     DAY HOURS
    JAN.       7.728         FEB.       9.314         MAR.       11.59
    APR.       14.04         MAY        15.93         JUNE       16.78
    JULY       16.33         AUG.       14.68         SEP.       12.33
    OCT.       9.890         NOV.       8.016         DEC.       7.221

 SNOW MELT COEFFICIENT [CM/DEG-C-DAY]               0.4600
 INITIAL CROP NUMBER                                    12
 INITIAL CROP CONDITION                                  1



NO CALCULATION OF RUNOFF EVENTS
 CROP INFORMATION
 ----------------

        MAXIMUM                                      IRRIGATION PERENNIAL TILLAGE   SURFACE
        INTERCEPT.MAXIMUM     MAXIMUM   MAXIMUM      FLAG    CROP        FLAG    CONDITION
USLE COVER MANAGEMENT
 CROP   POTENTIAL ROOT DEPTH  COVER     WEIGHT       (0=NO)  (0=NO)    (0=NO)    AFTER
AMC         RUNOFF CURVE NUMBERS     "C" FACTOR
```

NUMBER FALLOW	[CM] CROP	[CM] RESIDUE	[%] FALLOW	[KG/M**2] CROP	(1=YES) RESIDUE	(1=YES)	(1=YES)	HARVEST
I	72	51	72					
12	0.0000	100.0	90.00	0.0000	0	0	0	3
II	86	70	86	1.0000	1.0000	1.0000		
III	94	84	94					

CROP ROTATION INFORMATION

CROP NUMBER	TILLAGE DATE	EMERGENCE DATE	MATURATION DATE	SENESCENCE HARVEST DATE
Winter Rape		2 SEP., 1	5 MAY , 2	28 JUNE, 2 28 JULY, 2
Winter Rape		2 SEP., 2	5 MAY , 3	28 JUNE, 3 28 JULY, 3
Winter Rape		2 SEP., 3	5 MAY , 4	28 JUNE, 4 28 JULY, 4

*** PARAMETERS OF ACTIVE SUBSTANCE (Parent)***

PESTICIDE APPLICATION INFORMATION

APPLICATION DATE	PESTICIDE APPLIED [KG/HA]	INCORPORATION DEPTH [CM]
21 AUG., 1	1.200	0.0000

PLANT PESTICIDE PARAMETERS

MODEL UTILIZED (1=SOIL,2=LINEAR,3=EXPONENTIAL 1

VOLATILIZATION PARAMETERS ACTIVE SUBSTANCE

TEMPERATURE [deg C]	20.00
HENRY-CONSTANT [Pa*m3/mole] or [J/mole] CALCULATED USING	0.2000E-04
VAPOUR PRESSURE [Pa]	0.1000E-03
MOLECULAR MASS [g/mole]	100.0
WATER SOLUBILITY [mg/l]	500.0
TEMPERATURE [deg C]	30.00
HENRY-CONSTANT [Pa*m3/mole] or [J/mole] CALCULATED USING	0.4000E-04
VAPOUR PRESSURE [Pa]	0.4000E-03
MOLECULAR MASS [g/mole]	100.0
WATER SOLUBILITY [mg/l]	1000.
Q10-Factor for Henry's constant:	2.000
DIFFUSION COEFF.AIR [cm2/d]	4303.
DEPTH OF SURFACE LAYER FOR VOLATILIZATION [CM]	0.1000
HENRY CONSTANT AT 20.0 deg C [-]	0.8206E-08
HENRY CONSTANT AT 30.0 deg C [-]	0.1587E-07

PLANT UPTAKE OF ACTIVE SUBSTANCE

PLANT UPTAKE FACTOR (-)	0.0000

TRANSFORMATION PARAMETERS

TRANSFORM. TO	TRANSFORM. in EQ.Domaine [/DAY]	TEMP. OF STUDY [C]	Q10 VALUE [-]	MOISTURE-DURING-STUDY ABSOLUTE [%]	MOISTURE RELATIVE [%]	REL. TRANSFORM EXPONENT [-]	IN NEQ DOMAIN [-]
MET. A1	0.1000E-09	20.00	2.580	0.0000	100.0	0.7000	0.0000

MET. B1	0.1000E-09	20.00	2.580	0.0000	100.0	0.7000	0.0000
MET. C1	0.1000E-09	20.00	2.580	0.0000	100.0	0.7000	0.0000
MET. D1	0.1000E-09	20.00	2.000	19.00	0.0000	0.0000	0.0000
BR/CO2	0.3086E-01	20.00	2.580	0.0000	100.0	0.7000	0.0000

SORPTION PARAMETERS

--PARAMETERS TO CALCULATE KD-VALUES WITH KOC--

KOC [CM**3/G]	95.17
FREUNDLICH-SORPTION EXPONENT 1/n	0.9000
[PEARL] FACTOR DESCRIBING NON-EQ-SITES EQ-SITES (-):	0.0000
[PEARL] DESORPTION RATE [1/D]:	0.0000
MIN. CONC FOR FREUNDLICH-SORPTION [æG/L]	0.1000E-19

DEPTH DEPENDEND SORPTION AND TRANSFORMATION PARAMETERS

HORIZON	KOC	KD	FR-EXP	TRANSFORMATION RATE TO				
				MET. A1	MET. B1	MET. C1	MET. D1	BR/CO2
	[CM**3/G]	[CM**3/G]	[-]	[/DAY]	[/DAY]	[/DAY]	[/DAY]	[/DAY]
1	95.17	1.428	0.9000	0.1000E-09	0.1000E-09	0.1000E-09	0.1000E-09	0.3086E-01
2	95.17	0.9517	0.9000	0.5000E-10	0.5000E-10	0.5000E-10	0.5000E-10	0.1543E-01
3	95.17	0.1903	0.9000	0.3000E-10	0.3000E-10	0.3000E-10	0.3000E-10	0.9258E-02
4	0.0000	0.0000	0.9000	0.3000E-10	0.3000E-10	0.3000E-10	0.3000E-10	0.9258E-02
5	0.0000	0.0000	0.9000	0.3000E-10	0.3000E-10	0.3000E-10	0.3000E-10	0.9258E-02

Subs
Ver 3 Hamburg, oil seed rape (winter)

GENERAL SOIL INFORMATION

CORE DEPTH [CM]		100.0
TOTAL HORIZONS IN CORE		5
TOTAL COMPARTMENTS IN CORE		20
DPFLAG FLAG	(0=DISP.COEFF.1=DISP.LENGTH)	1
THETA FLAG	(0=INPUT,1=PRZM 2=PELMO)	0
PARTITION COEFFICIENT FLAG	(0=INPUT,1=CALCULATED)	1
BULK DENSITY FLAG	(0=INPUT,1=CALCULATED)	0
SOIL HYDRAULICS MODULE		free drainage

SOIL HORIZON INFORMATION

HORIZON	THICKNESS [CM]	BULK DENSITY [G/CM**3]	INITIAL SOIL WATER CONTENT [CM/CM]	DRAINAGE PARAMETER [/DAY]	FIELD CAPACITY WATER CONTENT [CM/CM]	WILTING POINT WATER CONTENT [CM/CM]	DISPERSION LENGTH [CM]	ORGANIC CARBON [%]	BIODEG. FACTOR [-]	PH [-]
1	30.0000	1.5000	0.2810	2.3000	0.2920	0.0640	5.0000	1.5000	1.0000	6.4000
2	30.0000	1.6000	0.2810	2.3000	0.2770	0.0470	5.0000	1.0000	0.5000	5.6000
3	15.0000	1.5600	0.2810	2.3000	0.2290	0.0400	5.0000	0.2000	0.3000	5.6000
4	15.0000	1.6200	0.2810	2.3000	0.1630	0.0220	5.0000	0.0000	0.3000	5.7000
5	10.0000	1.6000	0.2810	0.0000	0.1630	0.0220	5.0000	0.0000	0.3000	5.5000

OUTPUT FILE PARAMETERS

OUTPUT	TIME STEP	LAYER FREQ
WATR	DAY	1
PEST	DAY	1
CONC	DAY	1

Total number of layers in the top meter: 21

PLOT FILE INFORMATION

NUMBER OF PLOTTING VARIABLES 1

TIMSER NAME	MODE	DEPTH(CM)	ARGUMENT	CONSTANT	SUBSTANCE
LEAC	TSER	100.	21	0.1000E+10	PESTIC